OCTYL BENZOATE

Other names: 1-octyl benzoate
benzoic acid, octyl ester
n-Octyl benzoate
Inchi: InChI=1S/C15H22O2/c1-2-3-4-5-6-10-13-17-15(16)14-11-8-7-9-12-14/h7-9,11-12H,2-6,1
InchiKey: VECVSKFWRQYTAL-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
af	0.7482		Cheméo Relay (1.0)
hf	-412.01	kJ/mol	Cheméo Relay (1.0)
hfus	31.43	kJ/mol	Joback Method
hvap	79.72	kJ/mol	Cheméo Relay (1.0)
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-5.17		Cheméo Relay (1.0)
logp	4.204		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1778.79		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1778.79		NIST Webbook

rinpol	1792.23		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1774.00		NIST Webbook
ripol	2258.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2258.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2249.00		NIST Webbook
ripol	2284.00		NIST Webbook
ripol	2298.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2304.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2287.00		NIST Webbook
tb	532.55 ± 1.00	K	NIST Webbook
tc	771.78	K	Cheméo Relay (1.0)
tf	260.23	K	Cheméo Relay (1.0)
vc	0.778	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.39	J/mol×K	645.57	Joback Method
cpg	563.17	J/mol×K	678.49	Joback Method
cpg	579.02	J/mol×K	711.41	Joback Method
cpg	593.96	J/mol×K	744.32	Joback Method
cpg	608.02	J/mol×K	777.24	Joback Method
cpg	621.23	J/mol×K	810.16	Joback Method
cpg	633.62	J/mol×K	843.08	Joback Method
dvisc	0.0019370	Pa×s	357.39	Joback Method
dvisc	0.0009578	Pa×s	405.42	Joback Method
dvisc	0.0005498	Pa×s	453.45	Joback Method
dvisc	0.0003510	Pa×s	501.48	Joback Method
dvisc	0.0002424	Pa×s	549.51	Joback Method
dvisc	0.0001776	Pa×s	597.54	Joback Method

dvisc	0.0001364	Pa×s	645.57	Joback Method

Sources

Experimental Isobaric Vapor Liquid Equilibrium for Binary Systems Diethylene Glycol Dibenzoate + Diethylene Glycol, Diethylene Glycol Dibenzoate + Octyl Benzoate, and Ternary System Diethylene Glycol Dibenzoate + Diethylene Glycol + Octyl Benzoate at 1.0152 kPa:	https://www.doi.org/10.1021/acs.jced.8b00460
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94508&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume