

Phthalic acid, octyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C24H38O4/c1-6-7-8-9-10-13-16-27-22(25)20-14-11-12-15-21(20)23(26)28-18-
InchiKey:	JROSLADULBHD-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCCOC(=O)c1cccc1C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-213.46	kJ/mol	Joback Method
hf	-817.26	kJ/mol	Joback Method
hfus	46.20	kJ/mol	Joback Method
hvap	88.58	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.433		Crippen Method
mvol	340.140	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook
tb	929.09	K	Joback Method
tc	1140.66	K	Joback Method
tf	530.92	K	Joback Method
vc	1.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.03	J/molxK	929.09	Joback Method
cpg	1137.08	J/molxK	964.35	Joback Method
cpg	1152.82	J/molxK	999.61	Joback Method
cpg	1167.30	J/molxK	1034.87	Joback Method
cpg	1180.59	J/molxK	1070.14	Joback Method
cpg	1192.72	J/molxK	1105.40	Joback Method
cpg	1203.78	J/molxK	1140.66	Joback Method
dvisc	0.0003846	Paxs	530.92	Joback Method

dvisc	0.0001823	Paxs	597.28	Joback Method
dvisc	0.0001003	Paxs	663.64	Joback Method
dvisc	0.0000616	Paxs	730.00	Joback Method
dvisc	0.0000410	Paxs	796.37	Joback Method
dvisc	0.0000290	Paxs	862.73	Joback Method
dvisc	0.0000216	Paxs	929.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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