decyl benzoate

Other names: Benzoic acid, decyl ester
n-decyl benzoate
Inchi: InChI=1S/C17H26O2/c1-2-3-4-5-6-7-8-12-15-19-17(18)16-13-10-9-11-14-16/h9-11,13-14
InchiKey: CUSUFTNOPPMGBK-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 262.39
CAS: 36685-97-9

Physical Properties

Property code	Value	Unit	Source
gf	-29.25	kJ/mol	Joback Method
hf	-402.48	kJ/mol	Joback Method
hfus	36.61	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.984		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	1972.00		NIST Webbook
rinpol	1977.32		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1957.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1977.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1973.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1977.32		NIST Webbook
rinpol	1977.00		NIST Webbook

rinpol	2003.36		NIST Webbook
ripol	2494.00		NIST Webbook
ripol	2474.00		NIST Webbook
ripol	2500.00		NIST Webbook
ripol	2504.00		NIST Webbook
ripol	2475.00		NIST Webbook
ripol	2488.00		NIST Webbook
ripol	2506.00		NIST Webbook
ripol	2473.00		NIST Webbook
ripol	2473.00		NIST Webbook
ripol	2464.00		NIST Webbook
ripol	2486.00		NIST Webbook
ripol	2519.00		NIST Webbook
ripol	2519.00		NIST Webbook
ripol	2474.00		NIST Webbook
ripol	2506.00		NIST Webbook
tb	691.33	K	Joback Method
tc	884.75	K	Joback Method
tf	379.93	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.86	J/mol×K	691.33	Joback Method
cpg	672.36	J/mol×K	723.57	Joback Method
cpg	688.87	J/mol×K	755.80	Joback Method
cpg	704.44	J/mol×K	788.04	Joback Method
cpg	719.09	J/mol×K	820.27	Joback Method
cpg	732.85	J/mol×K	852.51	Joback Method
cpg	745.76	J/mol×K	884.75	Joback Method
dvisc	0.0016807	Pa×s	379.93	Joback Method
dvisc	0.0008086	Pa×s	431.83	Joback Method
dvisc	0.0004552	Pa×s	483.73	Joback Method
dvisc	0.0002864	Pa×s	535.63	Joback Method
dvisc	0.0001956	Pa×s	587.53	Joback Method
dvisc	0.0001421	Pa×s	639.43	Joback Method
dvisc	0.0001083	Pa×s	691.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36685979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume