

Hydratropic acid, tetradecyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C23H38O2/c1-3-4-5-6-7-8-9-10-11-12-13-17-20-25-23(24)21(2)22-18-15-14-16

WNIABVYAEVOKTE-UHFFFAOYSA-N

C23H38O2

CCCCCCCCCCCCCCCCOC(=O)C(C)c1ccccc1

346.55

Physical Properties

Property code	Value	Unit	Source
gf	18.83	kJ/mol	Joback Method
hf	-531.60	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	7.034		Crippen Method
mcvol	318.610	ml/mol	McGowan Method
pc	1081.35	kPa	Joback Method
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	828.17	K	Joback Method
tc	1022.35	K	Joback Method
tf	432.55	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.57	J/mol×K	828.17	Joback Method
cpg	1025.71	J/mol×K	860.53	Joback Method
cpg	1043.68	J/mol×K	892.90	Joback Method
cpg	1060.54	J/mol×K	925.26	Joback Method
cpg	1076.33	J/mol×K	957.62	Joback Method
cpg	1091.09	J/mol×K	989.99	Joback Method
cpg	1104.87	J/mol×K	1022.35	Joback Method
dvisc	0.0011302	Pa×s	432.55	Joback Method

dvisc	0.0004634	Pa×s	498.49	Joback Method
dvisc	0.0002340	Pa×s	564.42	Joback Method
dvisc	0.0001363	Pa×s	630.36	Joback Method
dvisc	0.0000880	Pa×s	696.30	Joback Method
dvisc	0.0000612	Pa×s	762.23	Joback Method
dvisc	0.0000452	Pa×s	828.17	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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