

Hydratropic acid, pentadecyl ester

Inchi:

InChI=1S/C24H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-21-26-24(25)22(2)23-19-16-15

InchiKey:

FMQQNODIOZUOIL-UHFFFAOYSA-N

Formula:

C24H40O2

SMILES:

CCCCCCCCCCCCCCCCOC(=O)C(C)c1ccccc1

Mol. weight [g/mol]:

360.57

Physical Properties

Property code	Value	Unit	Source
gf	27.25	kJ/mol	Joback Method
hf	-552.24	kJ/mol	Joback Method
hfus	51.22	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	7.425		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1016.18	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	851.05	K	Joback Method
tc	1047.04	K	Joback Method
tf	443.82	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.10	J/mol×K	851.05	Joback Method
cpg	1153.46	J/mol×K	1014.38	Joback Method
cpg	1138.59	J/mol×K	981.71	Joback Method
cpg	1122.67	J/mol×K	949.05	Joback Method
cpg	1105.65	J/mol×K	916.38	Joback Method
cpg	1087.47	J/mol×K	883.72	Joback Method
cpg	1167.33	J/mol×K	1047.04	Joback Method
dvisc	0.0000391	Pa×s	851.05	Joback Method

dvisc	0.0000532	Pa×s	783.18	Joback Method
dvisc	0.0000765	Pa×s	715.31	Joback Method
dvisc	0.0001190	Pa×s	647.43	Joback Method
dvisc	0.0002051	Pa×s	579.56	Joback Method
dvisc	0.0004084	Pa×s	511.69	Joback Method
dvisc	0.0010041	Pa×s	443.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415072&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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