

Hydratropic acid, heptadecyl ester

Inchi:	InChI=1S/C26H44O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-28-26(27)24(2)25-2
InchiKey:	RDBNXQRCHUYSTD-UHFFFAOYSA-N
Formula:	C26H44O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(C)c1cccc1
Mol. weight [g/mol]:	388.63

Physical Properties

Property code	Value	Unit	Source
gf	44.09	kJ/mol	Joback Method
hf	-593.52	kJ/mol	Joback Method
hfus	56.40	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	8.205		Crippen Method
mvol	360.880	ml/mol	McGowan Method
pc	902.34	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	896.81	K	Joback Method
tc	1098.81	K	Joback Method
tf	466.36	K	Joback Method
vc	1.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.14	J/molxK	896.81	Joback Method
cpg	1213.08	J/molxK	930.48	Joback Method
cpg	1231.72	J/molxK	964.14	Joback Method
cpg	1249.14	J/molxK	997.81	Joback Method
cpg	1265.37	J/molxK	1031.48	Joback Method
cpg	1280.49	J/molxK	1065.15	Joback Method
cpg	1294.55	J/molxK	1098.81	Joback Method
dvisc	0.0007843	Paxs	466.36	Joback Method

dvisc	0.0003143	Paxs	538.10	Joback Method
dvisc	0.0001562	Paxs	609.84	Joback Method
dvisc	0.0000900	Paxs	681.59	Joback Method
dvisc	0.0000575	Paxs	753.33	Joback Method
dvisc	0.0000398	Paxs	825.07	Joback Method
dvisc	0.0000292	Paxs	896.81	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U415074&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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