

Di-iso-amyl tartrate

Other names:	diisopentyl tartrate
Inchi:	InChI=1S/C14H26O6/c1-9(2)5-7-19-13(17)11(15)12(16)14(18)20-8-6-10(3)4/h9-12,15-16
InchiKey:	VOBHVQRBBHSZAZ-UHFFFAOYSA-N
Formula:	C14H26O6
SMILES:	CC(C)CCOC(=O)C(O)C(O)C(=O)OCCC(C)C
Mol. weight [g/mol]:	290.35
CAS:	16016-41-4

Physical Properties

Property code	Value	Unit	Source
gf	-684.24	kJ/mol	Joback Method
hf	-1147.47	kJ/mol	Joback Method
hfus	31.67	kJ/mol	Joback Method
hvap	96.88	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	0.887		Crippen Method
mcvol	234.740	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
tb	854.90	K	Joback Method
tc	1047.58	K	Joback Method
tf	453.50	K	Joback Method
vc	0.881	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.33	J/molxK	854.90	Joback Method
cpg	759.68	J/molxK	887.01	Joback Method
cpg	771.15	J/molxK	919.13	Joback Method
cpg	781.73	J/molxK	951.24	Joback Method
cpg	791.44	J/molxK	983.35	Joback Method
cpg	800.29	J/molxK	1015.47	Joback Method
cpg	808.28	J/molxK	1047.58	Joback Method
dvisc	0.0009996	Paxs	453.50	Joback Method

dvisc	0.0001848	Paxs	520.40	Joback Method
dvisc	0.0000502	Paxs	587.30	Joback Method
dvisc	0.0000178	Paxs	654.20	Joback Method
dvisc	0.0000076	Paxs	721.10	Joback Method
dvisc	0.0000038	Paxs	788.00	Joback Method
dvisc	0.0000021	Paxs	854.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16016414&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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