

Di-isopropyl tartrate

Other names:	(+)-Diisopropyl tartrate
Inchi:	InChI=1S/C10H18O6/c1-5(2)15-9(13)7(11)8(12)10(14)16-6(3)4/h5-8,11-12H,1-4H3/t7-,8
InchiKey:	XEBCWEDRGPSHQH-YUMQZZPRSA-N
Formula:	C10H18O6
SMILES:	CC(C)OC(=O)C(O)C(O)C(=O)OC(C)C
Mol. weight [g/mol]:	234.25
CAS:	2217-15-4

Physical Properties

Property code	Value	Unit	Source
gf	-717.92	kJ/mol	Joback Method
hf	-1064.91	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	-0.389		Crippen Method
mcvol	178.380	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1385.20		NIST Webbook
rinpol	1385.20		NIST Webbook
tb	763.38	K	Joback Method
tc	946.82	K	Joback Method
tf	408.42	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.34	J/molxK	763.38	Joback Method
cpg	536.68	J/molxK	793.95	Joback Method
cpg	546.38	J/molxK	824.53	Joback Method
cpg	555.45	J/molxK	855.10	Joback Method
cpg	563.88	J/molxK	885.67	Joback Method
cpg	571.68	J/molxK	916.24	Joback Method

cpg	578.84	J/molxK	946.82	Joback Method
dvisc	0.0030290	Paxs	408.42	Joback Method
dvisc	0.0005379	Paxs	467.58	Joback Method
dvisc	0.0001408	Paxs	526.74	Joback Method
dvisc	0.0000483	Paxs	585.90	Joback Method
dvisc	0.0000202	Paxs	645.06	Joback Method
dvisc	0.0000098	Paxs	704.22	Joback Method
dvisc	0.0000053	Paxs	763.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.20	K	1.60	NIST Webbook

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=C2217154&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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