

dl-tropic acid

Inchi:	InChI=1S/C9H10O3/c10-6-8(9(11)12)7-4-2-1-3-5-7/h1-5,8,10H,6H2,(H,11,12)
InchiKey:	JACRWUWPXAESPB-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	O=C(O)C(CO)c1ccccc1
Mol. weight [g/mol]:	166.18

Physical Properties

Property code	Value	Unit	Source
gf	-267.69	kJ/mol	Joback Method
hf	-414.88	kJ/mol	Joback Method
hfus	19.36	kJ/mol	Joback Method
hvap	77.62	kJ/mol	Joback Method
log10ws	-0.93		Aqueous Solubility Prediction Method
logp	0.847		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
tb	669.79	K	Joback Method
tc	864.81	K	Joback Method
tf	374.18	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.39	J/molxK	669.79	Joback Method
cpg	364.51	J/molxK	832.31	Joback Method
cpg	357.90	J/molxK	799.80	Joback Method
cpg	350.81	J/molxK	767.30	Joback Method
cpg	343.21	J/molxK	734.80	Joback Method
cpg	335.08	J/molxK	702.29	Joback Method
cpg	370.66	J/molxK	864.81	Joback Method
dvisc	0.0000199	Paxs	669.79	Joback Method
dvisc	0.0000356	Paxs	620.52	Joback Method

dvisc	0.0000705	Paxs	571.25	Joback Method
dvisc	0.0001588	Paxs	521.99	Joback Method
dvisc	0.0004236	Paxs	472.72	Joback Method
dvisc	0.0014200	Paxs	423.45	Joback Method
dvisc	0.0065458	Paxs	374.18	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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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