

Citric acid, tripentyl ester

Inchi:	InChI=1S/C21H38O7/c1-4-7-10-13-26-18(22)16-21(25,20(24)28-15-12-9-6-3)17-19(23)2
InchiKey:	DXRFOGXSSDRZFP-UHFFFAOYSA-N
Formula:	C21H38O7
SMILES:	CCCCCOC(=O)CC(O)(CC(=O)OCCCCC)C(=O)OCCCCC
Mol. weight [g/mol]:	402.52
CAS:	70289-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-709.80	kJ/mol	Joback Method
hf	-1372.15	kJ/mol	Joback Method
hfus	55.18	kJ/mol	Joback Method
hvap	105.19	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.698		Crippen Method
mcvol	334.940	ml/mol	McGowan Method
pc	1122.31	kPa	Joback Method
tb	997.70	K	Joback Method
tc	1228.75	K	Joback Method
tf	606.15	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.49	J/molxK	997.70	Joback Method
cpg	1204.27	J/molxK	1190.24	Joback Method
cpg	1195.29	J/molxK	1151.73	Joback Method
cpg	1184.86	J/molxK	1113.23	Joback Method
cpg	1172.95	J/molxK	1074.72	Joback Method
cpg	1159.51	J/molxK	1036.21	Joback Method
cpg	1211.85	J/molxK	1228.75	Joback Method
dvisc	0.0000029	Paxs	997.70	Joback Method
dvisc	0.0000043	Paxs	932.44	Joback Method

dvisc	0.0000066	Paxs	867.18	Joback Method
dvisc	0.0000109	Paxs	801.92	Joback Method
dvisc	0.0000196	Paxs	736.67	Joback Method
dvisc	0.0000398	Paxs	671.41	Joback Method
dvisc	0.0000938	Paxs	606.15	Joback Method

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=C70289348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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