

Glutaric acid, 8-chlorooctyl 3,7-dimethyloctyl ester

Inchi:	InChI=1S/C23H43ClO4/c1-20(2)12-10-13-21(3)16-19-28-23(26)15-11-14-22(25)27-18-9
InchiKey:	XAYPYTQMLFXNLZ-UHFFFAOYSA-N
Formula:	C23H43ClO4
SMILES:	CC(C)CCCC(C)CCOC(=O)CCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	419.04

Physical Properties

Property code	Value	Unit	Source
gf	-341.87	kJ/mol	Joback Method
hf	-1033.95	kJ/mol	Joback Method
hfus	58.05	kJ/mol	Joback Method
hvap	88.71	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.675		Crippen Method
mvol	362.050	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	914.77	K	Joback Method
tc	1120.25	K	Joback Method
tf	493.21	K	Joback Method
vc	1.409	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.56	J/molxK	914.77	Joback Method
cpg	1266.11	J/molxK	1086.00	Joback Method
cpg	1252.82	J/molxK	1051.76	Joback Method
cpg	1238.26	J/molxK	1017.51	Joback Method
cpg	1222.38	J/molxK	983.26	Joback Method
cpg	1205.16	J/molxK	949.02	Joback Method
cpg	1278.15	J/molxK	1120.25	Joback Method
dvisc	0.0000241	Paxs	914.77	Joback Method

dvisc	0.0000330	Paxs	844.51	Joback Method
dvisc	0.0000478	Paxs	774.25	Joback Method
dvisc	0.0000747	Paxs	703.99	Joback Method
dvisc	0.0001287	Paxs	633.73	Joback Method
dvisc	0.0002543	Paxs	563.47	Joback Method
dvisc	0.0006097	Paxs	493.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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