

Glutaric acid, 10-chlorodecyl 8-chlorooctyl ester

Inchi:	InChI=1S/C23H42Cl2O4/c24-18-11-7-3-1-2-5-9-13-20-28-22(26)16-15-17-23(27)29-21-1
InchiKey:	FOFRDBGBNCCSAN-UHFFFAOYSA-N
Formula:	C23H42Cl2O4
SMILES:	O=C(CCCC(=O)OCCCCCCCCCCCCI)OCCCCCCCCCI
Mol. weight [g/mol]:	453.48

Physical Properties

Property code	Value	Unit	Source
gf	-348.92	kJ/mol	Joback Method
hf	-1039.13	kJ/mol	Joback Method
hfus	69.29	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	7.182		Crippen Method
mvol	374.290	ml/mol	McGowan Method
pc	861.00	kPa	Joback Method
rinpol	3303.00		NIST Webbook
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tb	953.08	K	Joback Method
tc	1169.74	K	Joback Method
tf	553.13	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1214.65	J/molxK	953.08	Joback Method
cpg	1232.45	J/molxK	989.19	Joback Method
cpg	1248.81	J/molxK	1025.30	Joback Method
cpg	1263.76	J/molxK	1061.41	Joback Method
cpg	1277.35	J/molxK	1097.52	Joback Method
cpg	1289.62	J/molxK	1133.63	Joback Method
cpg	1300.62	J/molxK	1169.74	Joback Method
dvisc	0.0003575	Paxs	553.13	Joback Method

dvisc	0.0001791	Paxs	619.79	Joback Method
dvisc	0.0001026	Paxs	686.45	Joback Method
dvisc	0.0000649	Paxs	753.11	Joback Method
dvisc	0.0000442	Paxs	819.76	Joback Method
dvisc	0.0000319	Paxs	886.42	Joback Method
dvisc	0.0000241	Paxs	953.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392476&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

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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