

Glutaric acid, 2-chloropropyl propyl ester

Inchi:	InChI=1S/C11H19ClO4/c1-3-7-15-10(13)5-4-6-11(14)16-8-9(2)12/h9H,3-8H2,1-2H3
InchiKey:	VGOUCTWNYLKRRRI-UHFFFAOYSA-N
Formula:	C11H19ClO4
SMILES:	CCCOC(=O)CCCC(=O)OCC(C)Cl
Mol. weight [g/mol]:	250.72

Physical Properties

Property code	Value	Unit	Source
gf	-440.47	kJ/mol	Joback Method
hf	-780.99	kJ/mol	Joback Method
hfus	30.49	kJ/mol	Joback Method
hvap	62.39	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.280		Crippen Method
mcvol	192.970	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpola	1686.00		NIST Webbook
tb	640.65	K	Joback Method
tc	826.62	K	Joback Method
tf	372.97	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.12	J/molxK	640.65	Joback Method
cpg	555.08	J/molxK	795.62	Joback Method
cpg	544.18	J/molxK	764.63	Joback Method
cpg	532.64	J/molxK	733.63	Joback Method
cpg	520.45	J/molxK	702.64	Joback Method
cpg	507.61	J/molxK	671.64	Joback Method
cpg	565.32	J/molxK	826.62	Joback Method
dvisc	0.0001461	Paxs	640.65	Joback Method
dvisc	0.0001910	Paxs	596.04	Joback Method

dvisc	0.0002607	Paxs	551.42	Joback Method
dvisc	0.0003758	Paxs	506.81	Joback Method
dvisc	0.0005815	Paxs	462.20	Joback Method
dvisc	0.0009877	Paxs	417.58	Joback Method
dvisc	0.0019043	Paxs	372.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359492&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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