

Glutaric acid, (2-chlorocyclohexyl)methyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C18H31ClO4/c1-4-16(13(2)3)23-18(21)11-7-10-17(20)22-12-14-8-5-6-9-15(14)
InchiKey:	KXYWEZNXLPHRPT-UHFFFAOYSA-N
Formula:	C18H31ClO4
SMILES:	CCC(OC(=O)CCCC(=O)OCC1CCCCC1Cl)C(C)C
Mol. weight [g/mol]:	346.89

Physical Properties

Property code	Value	Unit	Source
gf	-367.23	kJ/mol	Joback Method
hf	-896.77	kJ/mol	Joback Method
hfus	38.01	kJ/mol	Joback Method
hvap	77.70	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.475		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
tb	815.25	K	Joback Method
tc	1018.66	K	Joback Method
tf	440.00	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.39	J/molxK	815.25	Joback Method
cpg	899.51	J/molxK	849.15	Joback Method
cpg	916.29	J/molxK	883.05	Joback Method
cpg	931.74	J/molxK	916.95	Joback Method
cpg	945.88	J/molxK	950.85	Joback Method
cpg	958.73	J/molxK	984.75	Joback Method
cpg	970.29	J/molxK	1018.66	Joback Method
dvisc	0.0013677	Paxs	440.00	Joback Method
dvisc	0.0006081	Paxs	502.54	Joback Method
dvisc	0.0003235	Paxs	565.08	Joback Method

dvisc	0.0001952	Paxs	627.62	Joback Method
dvisc	0.0001291	Paxs	690.17	Joback Method
dvisc	0.0000914	Paxs	752.71	Joback Method
dvisc	0.0000683	Paxs	815.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405442&Units=SI

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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