

Glutaric acid, (2-chlorocyclohexyl)methyl hept-2-yl ester

Inchi:	InChI=1S/C19H33ClO4/c1-3-4-5-9-15(2)24-19(22)13-8-12-18(21)23-14-16-10-6-7-11-17
InchiKey:	YRFAQQBKVGKZJD-UHFFFAOYSA-N
Formula:	C19H33ClO4
SMILES:	CCCCC(C)OC(=O)CCCC(=O)OCC1CCCCC1Cl
Mol. weight [g/mol]:	360.92

Physical Properties

Property code	Value	Unit	Source
gf	-356.37	kJ/mol	Joback Method
hf	-912.13	kJ/mol	Joback Method
hfus	44.12	kJ/mol	Joback Method
hvap	80.32	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	5.010		Crippen Method
mvol	294.830	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	2461.00		NIST Webbook
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tb	838.57	K	Joback Method
tc	1039.94	K	Joback Method
tf	466.27	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.78	J/molxK	838.57	Joback Method
cpg	1017.46	J/molxK	1006.38	Joback Method
cpg	1004.74	J/molxK	972.82	Joback Method
cpg	990.74	J/molxK	939.26	Joback Method
cpg	975.42	J/molxK	905.69	Joback Method
cpg	958.77	J/molxK	872.13	Joback Method
cpg	1028.89	J/molxK	1039.94	Joback Method
dvisc	0.0000645	Paxs	838.57	Joback Method

dvisc	0.0000853	Paxs	776.52	Joback Method
dvisc	0.0001182	Paxs	714.47	Joback Method
dvisc	0.0001744	Paxs	652.42	Joback Method
dvisc	0.0002793	Paxs	590.37	Joback Method
dvisc	0.0004994	Paxs	528.32	Joback Method
dvisc	0.0010425	Paxs	466.27	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=U405445&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
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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