

Glutaric acid, (2-chlorocyclohexyl)methyl 3-chlorophenyl ester

Inchi:	InChI=1S/C18H22Cl2O4/c19-14-6-3-7-15(11-14)24-18(22)10-4-9-17(21)23-12-13-5-1-2-8
InchiKey:	BVWQOSDUKPUHMH-UHFFFAOYSA-N
Formula:	C18H22Cl2O4
SMILES:	O=C(CCCC(=O)Oc1cccc(Cl)c1)OCC1CCCCC1Cl
Mol. weight [g/mol]:	373.27

Physical Properties

Property code	Value	Unit	Source
gf	-271.50	kJ/mol	Joback Method
hf	-676.89	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	85.80	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.756		Crippen Method
mvol	269.220	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	2807.00		NIST Webbook
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tb	885.22	K	Joback Method
tc	1114.67	K	Joback Method
tf	538.86	K	Joback Method
vc	1.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.44	J/molxK	885.22	Joback Method
cpg	825.70	J/molxK	923.46	Joback Method
cpg	838.44	J/molxK	961.70	Joback Method
cpg	849.70	J/molxK	999.94	Joback Method
cpg	859.49	J/molxK	1038.19	Joback Method
cpg	867.84	J/molxK	1076.43	Joback Method
cpg	874.78	J/molxK	1114.67	Joback Method
dvisc	0.0006188	Paxs	538.86	Joback Method

dvisc	0.0003648	Paxs	596.59	Joback Method
dvisc	0.0002361	Paxs	654.31	Joback Method
dvisc	0.0001639	Paxs	712.04	Joback Method
dvisc	0.0001202	Paxs	769.77	Joback Method
dvisc	0.0000921	Paxs	827.49	Joback Method
dvisc	0.0000730	Paxs	885.22	Joback Method

Sources

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=U405450&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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