Glutaric acid, cyclohexylmethyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C18H22Cl2O4/c19-14-8-4-9-15(18(14)20)24-17(22)11-5-10-16(21)23-12-13-6-

InchiKey: NFQFUAZZFGTVRX-UHFFFAOYSA-N

Formula: C18H22Cl2O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)OCC1CCCCC1

Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-273.42	kJ/mol	Joback Method
hf	-668.02	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	86.77	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.193		Crippen Method
mcvol	269.220	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2768.00		NIST Webbook
rinpol	2768.00		NIST Webbook
tb	894.87	K	Joback Method
tc	1125.18	K	Joback Method
tf	555.62	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.69	J/mol×K	894.87	Joback Method
cpg	819.49	J/mol×K	933.25	Joback Method
cpg	831.82	J/mol×K	971.64	Joback Method
cpg	842.72	J/mol×K	1010.02	Joback Method
cpg	852.22	J/mol×K	1048.41	Joback Method
cpg	860.34	J/mol×K	1086.79	Joback Method
cpg	867.11	J/mol×K	1125.18	Joback Method
dvisc	0.0004838	Pa×s	555.62	Joback Method

dvisc	0.0002871	Pa×s	612.16	Joback Method
dvisc	0.0001861	Pa×s	668.70	Joback Method
dvisc	0.0001290	Pa×s	725.24	Joback Method
dvisc	0.0000943	Pa×s	781.79	Joback Method
dvisc	0.0000720	Pa×s	838.33	Joback Method
dvisc	0.0000568	Pa×s	894.87	Joback Method

Sources

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=U391991&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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