

Glutaric acid, 3,5-dichlorophenyl propyl ester

Inchi:	InChI=1S/C14H16Cl2O4/c1-2-6-19-13(17)4-3-5-14(18)20-12-8-10(15)7-11(16)9-12/h7-9H
InchiKey:	WMJBCNMLGIKOLS-UHFFFAOYSA-N
Formula:	C14H16Cl2O4
SMILES:	CCCOC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	319.18

Physical Properties

Property code	Value	Unit	Source
gf	-331.55	kJ/mol	Joback Method
hf	-639.78	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.022		Crippen Method
mcvol	223.720	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpola	2228.00		NIST Webbook
tb	783.80	K	Joback Method
tc	997.33	K	Joback Method
tf	503.16	K	Joback Method
vc	0.858	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.93	J/molxK	783.80	Joback Method
cpg	601.07	J/molxK	819.39	Joback Method
cpg	612.28	J/molxK	854.98	Joback Method
cpg	622.58	J/molxK	890.56	Joback Method
cpg	631.97	J/molxK	926.15	Joback Method
cpg	640.45	J/molxK	961.74	Joback Method
cpg	648.04	J/molxK	997.33	Joback Method
dvisc	0.0006262	Paxs	503.16	Joback Method
dvisc	0.0004009	Paxs	549.93	Joback Method

dvisc	0.0002752	Paxs	596.71	Joback Method
dvisc	0.0001996	Paxs	643.48	Joback Method
dvisc	0.0001511	Paxs	690.25	Joback Method
dvisc	0.0001186	Paxs	737.03	Joback Method
dvisc	0.0000958	Paxs	783.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359438&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

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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