

Glutaric acid, 2,3-dichlorophenyl ethyl ester

Inchi:	InChI=1S/C13H14Cl2O4/c1-2-18-11(16)7-4-8-12(17)19-10-6-3-5-9(14)13(10)15/h3,5-6H
InchiKey:	IIBUNKLATSTHNL-UHFFFAOYSA-N
Formula:	C13H14Cl2O4
SMILES:	CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	305.15

Physical Properties

Property code	Value	Unit	Source
gf	-339.97	kJ/mol	Joback Method
hf	-619.14	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	75.21	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.632		Crippen Method
mvol	209.630	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	2154.00		NIST Webbook
rinpol	2154.00		NIST Webbook
tb	760.92	K	Joback Method
tc	976.92	K	Joback Method
tf	491.89	K	Joback Method
vc	0.801	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.52	J/molxK	760.92	Joback Method
cpg	547.24	J/molxK	796.92	Joback Method
cpg	558.09	J/molxK	832.92	Joback Method
cpg	568.05	J/molxK	868.92	Joback Method
cpg	577.15	J/molxK	904.92	Joback Method
cpg	585.37	J/molxK	940.92	Joback Method
cpg	592.72	J/molxK	976.92	Joback Method
dvisc	0.0006803	Paxs	491.89	Joback Method

dvisc	0.0004416	Paxs	536.73	Joback Method
dvisc	0.0003064	Paxs	581.57	Joback Method
dvisc	0.0002240	Paxs	626.40	Joback Method
dvisc	0.0001708	Paxs	671.24	Joback Method
dvisc	0.0001347	Paxs	716.08	Joback Method
dvisc	0.0001092	Paxs	760.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359225&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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