Glutaric acid, 2,6-dichlorophenyl ethyl ester

Inchi: InChI=1S/C13H14Cl2O4/c1-2-18-11(16)7-4-8-12(17)19-13-9(14)5-3-6-10(13)15/h3,5-6H,
InchiKey: AACBPDFCHOUTLQ-UHFFFAOYSA-N
Formula: C13H14Cl2O4
SMILES: CCOC(=O)CCCC(=O)Oc1c(Cl)cccc1Cl
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
mcvol	209.630	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tb	760.92	K	Joback Method
tc	976.92	K	Joback Method
tf	491.89	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004416	Pa×s	536.73	Joback Method
dvisc	0.0003064	Pa×s	581.57	Joback Method
dvisc	0.0002240	Pa×s	626.40	Joback Method
dvisc	0.0001708	Pa×s	671.24	Joback Method
dvisc	0.0001347	Pa×s	716.08	Joback Method
dvisc	0.0001092	Pa×s	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=U358827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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