Glutaric acid, 2,5-dichlorophenyl propyl ester

Inchi: InChI=1S/C14H16Cl2O4/c1-2-8-19-13(17)4-3-5-14(18)20-12-9-10(15)6-7-11(12)16/h6-7,
InchiKey: XMOJJPSPLYDERT-UHFFFAOYSA-N
Formula: C14H16Cl2O4
SMILES: CCCOC(=O)CCCC(=O)Oc1cc(Cl)ccc1Cl
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
rinpol	2212.00		NIST Webbook
tb	783.80	K	Joback Method
tc	997.33	K	Joback Method
tf	503.16	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002752	Pa×s	596.71	Joback Method
dvisc	0.0001996	Pa×s	643.48	Joback Method
dvisc	0.0001511	Pa×s	690.25	Joback Method
dvisc	0.0001186	Pa×s	737.03	Joback Method
dvisc	0.0000958	Pa×s	783.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U358993&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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