Glutaric acid, 2,2-dichloroethyl 2,4-dichlorophenyl ester

Inchi: InChI=1S/C13H12Cl4O4/c14-8-4-5-10(9(15)6-8)21-13(19)3-1-2-12(18)20-7-11(16)17/h4-

InchiKey: BRKSJDZRXALKKW-UHFFFAOYSA-N

Formula: C13H12Cl4O4

SMILES: O=C(CCCC(=O)Oc1ccc(Cl)cc1Cl)OCC(Cl)Cl

Mol. weight [g/mol]: 374.04

Physical Properties

Property code	Value	Unit	Source
gf	-366.27	kJ/mol	Joback Method
hf	-655.90	kJ/mol	Joback Method
hfus	41.53	kJ/mol	Joback Method
hvap	83.60	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.416		Crippen Method
mcvol	234.110	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	835.34	K	Joback Method
tc	1060.85	K	Joback Method
tf	536.73	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.65	J/mol×K	835.34	Joback Method
cpg	588.33	J/mol×K	872.92	Joback Method
cpg	597.05	J/mol×K	910.51	Joback Method
cpg	604.84	J/mol×K	948.09	Joback Method
cpg	611.69	J/mol×K	985.68	Joback Method
cpg	617.63	J/mol×K	1023.26	Joback Method
cpg	622.65	J/mol×K	1060.85	Joback Method
dvisc	0.0005342	Pa×s	536.73	Joback Method

dvisc	0.0003364	Pa×s	586.50	Joback Method
dvisc	0.0002277	Pa×s	636.27	Joback Method
dvisc	0.0001631	Pa×s	686.03	Joback Method
dvisc	0.0001223	Pa×s	735.80	Joback Method
dvisc	0.0000950	Pa×s	785.57	Joback Method
dvisc	0.0000761	Pa×s	835.34	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=U391850&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