

Glutaric acid, 2,2-dichloroethyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C13H12Cl4O4/c14-8-3-1-4-9(13(8)17)21-12(19)6-2-5-11(18)20-7-10(15)16/h1,
InchiKey: FOMIMATVBOJTAR-UHFFFAOYSA-N
Formula: C13H12Cl4O4
SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)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	2512.00		NIST Webbook
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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/molxK	835.34	Joback Method
cpg	617.63	J/molxK	1023.26	Joback Method
cpg	611.69	J/molxK	985.68	Joback Method
cpg	604.84	J/molxK	948.09	Joback Method
cpg	597.05	J/molxK	910.51	Joback Method
cpg	588.33	J/molxK	872.92	Joback Method
cpg	622.65	J/molxK	1060.85	Joback Method
dvisc	0.0000761	Paxs	835.34	Joback Method

dvisc	0.0000950	Paxs	785.57	Joback Method
dvisc	0.0001223	Paxs	735.80	Joback Method
dvisc	0.0001631	Paxs	686.03	Joback Method
dvisc	0.0002277	Paxs	636.27	Joback Method
dvisc	0.0003364	Paxs	586.50	Joback Method
dvisc	0.0005342	Paxs	536.73	Joback Method

Sources

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=U391987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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