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

Inchi: InChI=1S/C13H13Cl2FO4/c14-9-3-1-4-10(13(9)15)20-12(18)6-2-5-11(17)19-8-7-16/h1,3-

InchiKey: ZJZHMOSTAYLORQ-UHFFFAOYSA-N

Formula: C13H13Cl2FO4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)OCCF

Mol. weight [g/mol]: 323.14

Physical Properties

Property code	Value	Unit	Source
gf	-534.78	kJ/mol	Joback Method
hf	-815.25	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.582		Crippen Method
mcvol	211.400	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	760.19	K	Joback Method
tc	968.60	K	Joback Method
tf	492.48	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.30	J/mol×K	760.19	Joback Method
cpg	554.52	J/mol×K	794.92	Joback Method
cpg	564.91	J/mol×K	829.66	Joback Method
cpg	574.49	J/mol×K	864.39	Joback Method
cpg	583.24	J/mol×K	899.13	Joback Method
cpg	591.18	J/mol×K	933.86	Joback Method
cpg	598.31	J/mol×K	968.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393717&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
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