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

Inchi: InChI=1S/C14H11Cl2F5O4/c15-8-3-1-4-9(12(8)16)25-11(23)6-2-5-10(22)24-7-13(17,18)1

InchiKey: CRXIAJPOCZOWJY-UHFFFAOYSA-N

Formula: C14H11Cl2F5O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 409.13

Physical Properties

Property code	Value	Unit	Source
gf	-1299.92	kJ/mol	Joback Method
hf	-1637.83	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	70.76	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.810		Crippen Method
mcvol	232.570	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	773.69	K	Joback Method
tc	970.47	K	Joback Method
tf	510.95	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.92	J/mol×K	773.69	Joback Method
cpg	642.06	J/mol×K	806.49	Joback Method
cpg	651.40	J/mol×K	839.28	Joback Method
cpg	659.97	J/mol×K	872.08	Joback Method
cpg	667.82	J/mol×K	904.88	Joback Method
cpg	674.98	J/mol×K	937.67	Joback Method
cpg	681.51	J/mol×K	970.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393678&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