Glutaric acid, 2,3-dichlorophenyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C15H12Cl2F6O4/c16-8-3-1-4-9(12(8)17)27-11(25)6-2-5-10(24)26-7-14(19,20)1

InchiKey: KZTRKUWBOQTBTE-UHFFFAOYSA-N

Formula: C15H12Cl2F6O4

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

Mol. weight [g/mol]: 441.15

Physical Properties

Property code	Value	Unit	Source
gf	-1488.75	kJ/mol	Joback Method
hf	-1859.86	kJ/mol	Joback Method
hfus	41.97	kJ/mol	Joback Method
hvap	71.78	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.148		Crippen Method
mcvol	248.430	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
tb	795.40	K	Joback Method
tc	989.09	K	Joback Method
tf	507.81	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.61	J/mol×K	795.40	Joback Method
cpg	703.91	J/mol×K	827.68	Joback Method
cpg	713.40	J/mol×K	859.96	Joback Method
cpg	722.10	J/mol×K	892.25	Joback Method
cpg	730.07	J/mol×K	924.53	Joback Method
cpg	737.34	J/mol×K	956.81	Joback Method
cpg	743.97	J/mol×K	989.09	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=U393695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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