Glutaric acid, 2,4,6-trichlorophenyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C14H10Cl3F5O4/c15-7-4-8(16)12(9(17)5-7)26-11(24)3-1-2-10(23)25-6-13(18,1

InchiKey: QANVWSTXKUHZCG-UHFFFAOYSA-N

Formula: C14H10Cl3F5O4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 443.58

Physical Properties

Property code	Value	Unit	Source
gf	-1321.48	kJ/mol	Joback Method
hf	-1665.04	kJ/mol	Joback Method
hfus	43.63	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.463		Crippen Method
mcvol	244.810	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook
tb	816.10	K	Joback Method
tc	1018.08	K	Joback Method
tf	553.39	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.48	J/mol×K	816.10	Joback Method
cpg	660.55	J/mol×K	849.76	Joback Method
cpg	668.84	J/mol×K	883.43	Joback Method
cpg	676.39	J/mol×K	917.09	Joback Method
cpg	683.24	J/mol×K	950.76	Joback Method
cpg	689.44	J/mol×K	984.42	Joback Method
cpg	695.02	J/mol×K	1018.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393680&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