Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C17H15ClF8O4/c1-9-5-6-10(18)11(7-9)30-13(28)4-2-3-12(27)29-8-15(21,22)17

InchiKey: HBZIRZAMLPGTPT-UHFFFAOYSA-N

Formula: C17H15ClF8O4

SMILES: Cc1ccc(Cl)c(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1

Mol. weight [g/mol]: 470.74

Physical Properties

Property code	Value	Unit	Source
gf	-1846.76	kJ/mol	Joback Method
hf	-2286.37	kJ/mol	Joback Method
hfus	41.70	kJ/mol	Joback Method
hvap	68.92	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.438		Crippen Method
mcvol	267.910	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	799.04	K	Joback Method
tc	985.96	K	Joback Method
tf	504.03	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.46	J/mol×K	799.04	Joback Method
cpg	807.89	J/mol×K	830.19	Joback Method
cpg	818.47	J/mol×K	861.35	Joback Method
cpg	828.24	J/mol×K	892.50	Joback Method
cpg	837.26	J/mol×K	923.65	Joback Method
cpg	845.60	J/mol×K	954.80	Joback Method
cpg	853.30	J/mol×K	985.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393415&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

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