Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C16H12Cl2F8O4/c17-8-3-1-4-9(18)12(8)30-11(28)6-2-5-10(27)29-7-14(21,22)1

InchiKey: PNZRYVQPDLTCQP-UHFFFAOYSA-N

Formula: C16H12Cl2F8O4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cccc1Cl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 491.16

Physical Properties

Property code	Value	Unit	Source
gf	-1867.11	kJ/mol	Joback Method
hf	-2281.47	kJ/mol	Joback Method
hfus	43.30	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.783		Crippen Method
mcvol	266.060	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	813.59	K	Joback Method
tc	1004.64	K	Joback Method
tf	522.68	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.88	J/mol×K	813.59	Joback Method
cpg	774.93	J/mol×K	845.43	Joback Method
cpg	784.17	J/mol×K	877.27	Joback Method
cpg	792.66	J/mol×K	909.11	Joback Method
cpg	800.45	J/mol×K	940.96	Joback Method
cpg	807.61	J/mol×K	972.80	Joback Method
cpg	814.19	J/mol×K	1004.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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