

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

Inchi:	InChI=1S/C16H12Cl2F8O4/c17-8-4-5-10(9(18)6-8)30-12(28)3-1-2-11(27)29-7-14(21,22)
InchiKey:	UITPKYZGHAIJIH-UHFFFAOYSA-N
Formula:	C16H12Cl2F8O4
SMILES:	O=C(CCCC(=O)Oc1ccc(Cl)cc1Cl)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	2150.00		NIST Webbook
rinpol	2150.00		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/molxK	813.59	Joback Method
cpg	774.93	J/molxK	845.43	Joback Method
cpg	784.17	J/molxK	877.27	Joback Method
cpg	792.66	J/molxK	909.11	Joback Method
cpg	800.45	J/molxK	940.96	Joback Method
cpg	807.61	J/molxK	972.80	Joback Method
cpg	814.19	J/molxK	1004.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U391845&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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