

Fumaric acid, 2-chlorophenyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C15H9ClF8O4/c16-8-3-1-2-4-9(8)28-11(26)6-5-10(25)27-7-13(19,20)15(23,24)
InchiKey: RKDJOMPGENWKEY-AATRIKPKSA-N
Formula: C15H9ClF8O4
SMILES: O=C(C=CC(=O)Oc1ccccc1Cl)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)
Mol. weight [g/mol]: 440.67

Physical Properties

Property code	Value	Unit	Source
gf	-1773.75	kJ/mol	Joback Method
hf	-2116.40	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.516		Crippen Method
mvol	235.430	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	752.46	K	Joback Method
tc	940.99	K	Joback Method
tf	463.89	K	Joback Method
vc	0.950	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.69	J/molxK	752.46	Joback Method
cpg	674.81	J/molxK	783.88	Joback Method
cpg	684.11	J/molxK	815.30	Joback Method
cpg	692.67	J/molxK	846.73	Joback Method
cpg	700.54	J/molxK	878.15	Joback Method
cpg	707.80	J/molxK	909.57	Joback Method
cpg	714.51	J/molxK	940.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405719&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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