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

Inchi: InChI=1S/C15H18F8O4/c1-9(2)4-3-7-26-10(24)5-6-11(25)27-8-13(18,19)15(22,23)14(20

InchiKey: JADRWXAMLNKKKK-AATRIKPKSA-N

Formula: C15H18F8O4

SMILES: CC(C)CCCOC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 414.29

Physical Properties

Property code	Value	Unit	Source
gf	-1867.04	kJ/mol	Joback Method
hf	-2331.00	kJ/mol	Joback Method
hfus	35.73	kJ/mol	Joback Method
hvap	56.05	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.236		Crippen Method
mcvol	246.950	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	1625.00		NIST Webbook
rinpol	1625.00		NIST Webbook
tb	682.93	K	Joback Method
tc	846.80	K	Joback Method
tf	380.03	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.13	J/mol×K	682.93	Joback Method
cpg	739.39	J/mol×K	710.24	Joback Method
cpg	751.87	J/mol×K	737.55	Joback Method
cpg	763.59	J/mol×K	764.86	Joback Method
cpg	774.61	J/mol×K	792.18	Joback Method
cpg	784.96	J/mol×K	819.49	Joback Method
cpg	794.69	J/mol×K	846.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348781&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