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

Inchi: InChI=1S/C15H9F8NO6/c16-12(17)14(20,21)15(22,23)13(18,19)7-29-10(25)5-6-11(26)3

InchiKey: PZDUQUDRWYMOKB-AATRIKPKSA-N

Formula: C15H9F8NO6

SMILES: O=C(C=CC(=O)Oc1ccc([N+](=O)[O-])cc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 451.22

Physical Properties

Property code	Value	Unit	Source
gf	-1726.27	kJ/mol	Joback Method
hf	-2111.42	kJ/mol	Joback Method
hfus	44.27	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.771		Crippen Method
mcvol	240.610	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2183.00		NIST Webbook
tb	866.87	K	Joback Method
tc	1073.87	K	Joback Method
tf	577.58	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.08	J/mol×K	866.87	Joback Method
cpg	742.78	J/mol×K	901.37	Joback Method
cpg	750.73	J/mol×K	935.87	Joback Method
cpg	758.02	J/mol×K	970.37	Joback Method
cpg	764.74	J/mol×K	1004.87	Joback Method
cpg	770.98	J/mol×K	1039.37	Joback Method
cpg	776.83	J/mol×K	1073.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405787&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
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