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

Inchi: InChI=1S/C16H9F8NO4/c17-13(18)15(21,22)16(23,24)14(19,20)8-28-11(26)5-6-12(27)2

InchiKey: YWWQNIOXWMDAPP-AATRIKPKSA-N

Formula: C16H9F8NO4

SMILES: N#Cc1ccc(OC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)cc1

Mol. weight [g/mol]: 431.23

Physical Properties

Property code	Value	Unit	Source
gf	-1620.22	kJ/mol	Joback Method
hf	-1956.42	kJ/mol	Joback Method
hfus	37.00	kJ/mol	Joback Method
hvap	72.08	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	3.734		Crippen Method
mcvol	238.660	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	839.99	K	Joback Method
tc	1039.13	K	Joback Method
tf	510.23	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.28	J/mol×K	839.99	Joback Method
cpg	718.07	J/mol×K	873.18	Joback Method
cpg	726.14	J/mol×K	906.37	Joback Method
cpg	733.56	J/mol×K	939.56	Joback Method
cpg	740.41	J/mol×K	972.75	Joback Method
cpg	746.77	J/mol×K	1005.94	Joback Method
cpg	752.71	J/mol×K	1039.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405730&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

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