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

Inchi: InChI=1S/C17H22F8O4/c1-2-3-4-5-6-7-10-28-12(26)8-9-13(27)29-11-15(20,21)17(24,25)

InchiKey: ZFHSDWFPYFFSQU-CMDGGOBGSA-N

Formula: C17H22F8O4

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

Mol. weight [g/mol]: 442.34

Physical Properties

Property code	Value	Unit	Source
gf	-1847.76	kJ/mol	Joback Method
hf	-2367.00	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.160		Crippen Method
mcvol	275.130	ml/mol	McGowan Method
pc	1110.37	kPa	Joback Method
rinpol	1861.00		NIST Webbook
tb	729.13	K	Joback Method
tc	896.16	K	Joback Method
tf	417.57	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.46	J/mol×K	729.13	Joback Method
cpg	849.52	J/mol×K	756.97	Joback Method
cpg	862.74	J/mol×K	784.81	Joback Method
cpg	875.19	J/mol×K	812.65	Joback Method
cpg	886.90	J/mol×K	840.48	Joback Method
cpg	897.94	J/mol×K	868.32	Joback Method
cpg	908.34	J/mol×K	896.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348784&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