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

Inchi: InChI=1S/C27H42F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-38-22(36)18-19

InchiKey: IXTVOXNTQCCHAU-VHEBQXMUSA-N

Formula: C27H42F8O4

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

Mol. weight [g/mol]: 582.61

Physical Properties

Property code	Value	Unit	Source
gf	-1763.56	kJ/mol	Joback Method
hf	-2573.40	kJ/mol	Joback Method
hfus	70.34	kJ/mol	Joback Method
hvap	83.15	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	9.062		Crippen Method
mcvol	416.030	ml/mol	McGowan Method
pc	637.37	kPa	Joback Method
rinpol	2793.00		NIST Webbook
tb	957.93	K	Joback Method
tc	1198.54	K	Joback Method
tf	530.27	K	Joback Method
vc	1.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1435.74	J/mol×K	957.93	Joback Method
cpg	1457.23	J/mol×K	998.03	Joback Method
cpg	1477.27	J/mol×K	1038.13	Joback Method
cpg	1496.03	J/mol×K	1078.23	Joback Method
cpg	1513.73	J/mol×K	1118.33	Joback Method
cpg	1530.53	J/mol×K	1158.44	Joback Method
cpg	1546.64	J/mol×K	1198.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348794&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