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

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

InchiKey: BDLQSDCMIZUYQZ-CMDGGOBGSA-N

Formula: C17H22F8O4

SMILES: CCCCCCC(C)OC(=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	-1850.20	kJ/mol	Joback Method
hf	-2372.28	kJ/mol	Joback Method
hfus	40.91	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.159		Crippen Method
mcvol	275.130	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook
tb	728.69	K	Joback Method
tc	896.59	K	Joback Method
tf	402.57	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.97	J/mol×K	728.69	Joback Method
cpg	850.12	J/mol×K	756.67	Joback Method
cpg	863.42	J/mol×K	784.66	Joback Method
cpg	875.93	J/mol×K	812.64	Joback Method
cpg	887.69	J/mol×K	840.62	Joback Method
cpg	898.76	J/mol×K	868.61	Joback Method
cpg	909.18	J/mol×K	896.59	Joback Method

Sources

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=U405584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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