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

Inchi: InChI=1S/C17H22F8O4/c1-10(7-14(2,3)4)8-28-11(26)5-6-12(27)29-9-15(20,21)17(24,25)

InchiKey: JZTCSECCKLVUCI-AATRIKPKSA-N

Formula: C17H22F8O4

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

Mol. weight [g/mol]: 442.34

Physical Properties

Property code	Value	Unit	Source
gf	-1847.36	kJ/mol	Joback Method
hf	-2381.03	kJ/mol	Joback Method
hfus	33.50	kJ/mol	Joback Method
hvap	59.21	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.872		Crippen Method
mcvol	275.130	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
tb	725.46	K	Joback Method
tc	896.21	K	Joback Method
tf	404.99	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.14	J/mol×K	725.46	Joback Method
cpg	852.33	J/mol×K	753.92	Joback Method
cpg	865.62	J/mol×K	782.38	Joback Method
cpg	878.09	J/mol×K	810.83	Joback Method
cpg	889.78	J/mol×K	839.29	Joback Method
cpg	900.77	J/mol×K	867.75	Joback Method
cpg	911.12	J/mol×K	896.21	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=U405599&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