Fumaric acid, 2-octyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C15H22F4O4/c1-3-4-5-6-7-11(2)23-13(21)9-8-12(20)22-10-15(18,19)14(16)17
InchiKey: MFTHTHWQENCTBD-CMDGGOBGSA-N
Formula: C15H22F4O4
SMILES: CCCCCCC(C)OC(=O)C=CC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 342.33

Physical Properties

Property code	Value	Unit	Source
gf	-1093.48	kJ/mol	Joback Method
hf	-1529.06	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.888		Crippen Method
mcvol	239.870	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	692.31	K	Joback Method
tc	863.21	K	Joback Method
tf	372.83	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.47	J/mol×K	692.31	Joback Method
cpg	703.87	J/mol×K	720.79	Joback Method
cpg	717.51	J/mol×K	749.28	Joback Method
cpg	730.40	J/mol×K	777.76	Joback Method
cpg	742.59	J/mol×K	806.24	Joback Method
cpg	754.08	J/mol×K	834.73	Joback Method
cpg	764.91	J/mol×K	863.21	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=U405583&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