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

Inchi: InChI=1S/C11H10F8O4/c1-2-22-6(20)3-4-7(21)23-5-9(14,15)11(18,19)10(16,17)8(12)13/

InchiKey: RECSWTWQJZPFQW-ONEGZZNKSA-N

Formula: C11H10F8O4

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

Mol. weight [g/mol]: 358.18

Physical Properties

Property code	Value	Unit	Source
gf	-1898.28	kJ/mol	Joback Method
hf	-2243.16	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	47.54	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.820		Crippen Method
mcvol	190.590	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	591.85	K	Joback Method
tc	751.14	K	Joback Method
tf	349.95	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.10	J/mol×K	591.85	Joback Method
cpg	531.35	J/mol×K	618.40	Joback Method
cpg	541.91	J/mol×K	644.95	Joback Method
cpg	551.80	J/mol×K	671.49	Joback Method
cpg	561.07	J/mol×K	698.04	Joback Method
cpg	569.74	J/mol×K	724.59	Joback Method
cpg	577.85	J/mol×K	751.14	Joback Method

Sources

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=U348778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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