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

Inchi: InChI=1S/C13H14F8O4/c1-2-3-6-24-8(22)4-5-9(23)25-7-11(16,17)13(20,21)12(18,19)10(

InchiKey: KVOBWNUTDXYASP-SNAWJCMRSA-N

Formula: C13H14F8O4

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

Mol. weight [g/mol]: 386.24

Physical Properties

Property code	Value	Unit	Source
gf	-1881.44	kJ/mol	Joback Method
hf	-2284.44	kJ/mol	Joback Method
hfus	34.08	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.600		Crippen Method
mcvol	218.770	ml/mol	McGowan Method
pc	1460.13	kPa	Joback Method
rinpol	1496.00		NIST Webbook
tb	637.61	K	Joback Method
tc	797.65	K	Joback Method
tf	372.49	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.32	J/mol×K	637.61	Joback Method
cpg	632.54	J/mol×K	664.28	Joback Method
cpg	644.02	J/mol×K	690.96	Joback Method
cpg	654.82	J/mol×K	717.63	Joback Method
cpg	664.95	J/mol×K	744.31	Joback Method
cpg	674.47	J/mol×K	770.98	Joback Method
cpg	683.40	J/mol×K	797.65	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=U348779&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