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

Inchi: InChI=1S/C13H18F4O4/c1-3-9(4-2)7-20-10(18)5-6-11(19)21-8-13(16,17)12(14)15/h5-6,9

InchiKey: NGWZROIBSBOSHB-AATRIKPKSA-N

Formula: C13H18F4O4

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

Mol. weight [g/mol]: 314.27

Physical Properties

Property code	Value	Unit	Source
gf	-1110.32	kJ/mol	Joback Method
hf	-1487.78	kJ/mol	Joback Method
hfus	33.06	kJ/mol	Joback Method
hvap	57.46	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.966		Crippen Method
mcvol	211.690	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook
tb	646.55	K	Joback Method
tc	816.97	K	Joback Method
tf	350.29	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.70	J/mol×K	646.55	Joback Method
cpg	596.14	J/mol×K	674.95	Joback Method
cpg	608.87	J/mol×K	703.36	Joback Method
cpg	620.93	J/mol×K	731.76	Joback Method
cpg	632.33	J/mol×K	760.16	Joback Method
cpg	643.08	J/mol×K	788.57	Joback Method
cpg	653.23	J/mol×K	816.97	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=U405629&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

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