Fumaric acid, 2-ethylhexyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C15H23F3O4/c1-4-6-7-12(5-2)10-21-13(19)8-9-14(20)22-11(3)15(16,17)18/h8-

InchiKey: JVUVRLBFZQCDSG-CMDGGOBGSA-N

Formula: C15H23F3O4

SMILES: CCCCC(CC)COC(=O)C=CC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 324.34

Physical Properties

Property code	Value	Unit	Source
gf	-898.67	kJ/mol	Joback Method
hf	-1332.95	kJ/mol	Joback Method
hfus	35.16	kJ/mol	Joback Method
hvap	62.73	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.796		Crippen Method
mcvol	238.100	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	693.04	K	Joback Method
tc	868.58	K	Joback Method
tf	372.24	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.61	J/mol×K	693.04	Joback Method
cpg	696.46	J/mol×K	722.30	Joback Method
cpg	710.51	J/mol×K	751.55	Joback Method
cpg	723.79	J/mol×K	780.81	Joback Method
cpg	736.32	J/mol×K	810.07	Joback Method
cpg	748.14	J/mol×K	839.32	Joback Method
cpg	759.26	J/mol×K	868.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405569&Units=SI
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

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