Fumaric acid, 2-(2-methoxyethyl)hexyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H24F4O5/c1-3-4-5-12(8-9-23-2)10-24-13(21)6-7-14(22)25-11-16(19,20)15

InchiKey: KEWYYUGILYQIRG-VOTSOKGWSA-N

Formula: C16H24F4O5

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

Mol. weight [g/mol]: 372.35

Physical Properties

Property code	Value	Unit	Source
gf	-1190.06	kJ/mol	Joback Method
hf	-1681.92	kJ/mol	Joback Method
hfus	42.02	kJ/mol	Joback Method
hvap	66.55	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.372		Crippen Method
mcvol	259.830	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	737.61	K	Joback Method
tc	911.27	K	Joback Method
tf	406.33	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.64	J/mol×K	737.61	Joback Method
cpg	788.32	J/mol×K	766.55	Joback Method
cpg	802.18	J/mol×K	795.50	Joback Method
cpg	815.25	J/mol×K	824.44	Joback Method
cpg	827.54	J/mol×K	853.39	Joback Method
cpg	839.07	J/mol×K	882.33	Joback Method
cpg	849.86	J/mol×K	911.27	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=U405891&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