Diethylmalonic acid, hexyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H26F4O4/c1-4-7-8-9-10-23-13(21)15(5-2,6-3)14(22)24-11-16(19,20)12(17)

InchiKey: IRSZJBCSGQGHKA-UHFFFAOYSA-N

Formula: C16H26F4O4

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

Mol. weight [g/mol]: 358.37

Physical Properties

Property code	Value	Unit	Source
gf	-1160.00	kJ/mol	Joback Method
hf	-1670.39	kJ/mol	Joback Method
hfus	36.74	kJ/mol	Joback Method
hvap	63.27	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.360		Crippen Method
mcvol	258.260	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	1569.00		NIST Webbook
rinpol	1569.00		NIST Webbook
tb	708.24	K	Joback Method
tc	878.99	K	Joback Method
tf	406.60	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.44	J/mol×K	708.24	Joback Method
cpg	784.86	J/mol×K	736.70	Joback Method
cpg	799.45	J/mol×K	765.16	Joback Method
cpg	813.22	J/mol×K	793.62	Joback Method
cpg	826.21	J/mol×K	822.08	Joback Method
cpg	838.45	J/mol×K	850.54	Joback Method
cpg	849.96	J/mol×K	878.99	Joback Method

Sources

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=U370834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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