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

Inchi: InChI=1S/C16H25F5O4/c1-4-7-8-9-10-24-12(22)14(5-2,6-3)13(23)25-11-15(17,18)16(19

InchiKey: WBFNQJHEWSEJQO-UHFFFAOYSA-N

Formula: C16H25F5O4

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

Mol. weight [g/mol]: 376.36

Physical Properties

Property code	Value	Unit	Source
gf	-1349.53	kJ/mol	Joback Method
hf	-1869.97	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	61.55	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.657		Crippen Method
mcvol	260.030	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	704.72	K	Joback Method
tc	874.31	K	Joback Method
tf	424.61	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.01	J/mol×K	704.72	Joback Method
cpg	794.06	J/mol×K	732.98	Joback Method
cpg	808.25	J/mol×K	761.25	Joback Method
cpg	821.63	J/mol×K	789.51	Joback Method
cpg	834.23	J/mol×K	817.78	Joback Method
cpg	846.10	J/mol×K	846.04	Joback Method
cpg	857.28	J/mol×K	874.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370843&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

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