Diethylmalonic acid, hexyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C16H27F3O4/c1-5-8-9-10-11-22-13(20)15(6-2,7-3)14(21)23-12(4)16(17,18)19/

InchiKey: DMYOAENQOJHBPG-UHFFFAOYSA-N

Formula: C16H27F3O4

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

Mol. weight [g/mol]: 340.38

Physical Properties

Property code	Value	Unit	Source
gf	-965.19	kJ/mol	Joback Method
hf	-1474.28	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.410		Crippen Method
mcvol	256.490	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	708.97	K	Joback Method
tc	883.85	K	Joback Method
tf	406.01	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.65	J/mol×K	708.97	Joback Method
cpg	777.51	J/mol×K	738.12	Joback Method
cpg	792.49	J/mol×K	767.26	Joback Method
cpg	806.63	J/mol×K	796.41	Joback Method
cpg	819.95	J/mol×K	825.55	Joback Method
cpg	832.50	J/mol×K	854.70	Joback Method
cpg	844.30	J/mol×K	883.85	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=U370818&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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