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

Inchi: InChI=1S/C15H25F3O4/c1-5-8-9-10-21-12(19)14(6-2,7-3)13(20)22-11(4)15(16,17)18/h1

InchiKey: PAZYBNWGBUHWKI-UHFFFAOYSA-N

Formula: C15H25F3O4

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

Mol. weight [g/mol]: 326.35

Physical Properties

Property code	Value	Unit	Source
gf	-973.61	kJ/mol	Joback Method
hf	-1453.64	kJ/mol	Joback Method
hfus	31.07	kJ/mol	Joback Method
hvap	61.86	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.020		Crippen Method
mcvol	242.400	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	1425.00		NIST Webbook
rinpol	1425.00		NIST Webbook
tb	686.09	K	Joback Method
tc	860.62	K	Joback Method
tf	394.74	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.07	J/mol×K	686.09	Joback Method
cpg	721.54	J/mol×K	715.18	Joback Method
cpg	736.17	J/mol×K	744.27	Joback Method
cpg	749.98	J/mol×K	773.35	Joback Method
cpg	763.01	J/mol×K	802.44	Joback Method
cpg	775.28	J/mol×K	831.53	Joback Method
cpg	786.81	J/mol×K	860.62	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=U370817&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