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

Inchi: InChI=1S/C13H19F5O4/c1-4-7-21-9(19)11(5-2,6-3)10(20)22-8-12(14,15)13(16,17)18/h4-

InchiKey: LSHAEGYZNQABIS-UHFFFAOYSA-N

Formula: C13H19F5O4

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

Mol. weight [g/mol]: 334.28

Physical Properties

Property code	Value	Unit	Source
gf	-1374.79	kJ/mol	Joback Method
hf	-1808.05	kJ/mol	Joback Method
hfus	28.16	kJ/mol	Joback Method
hvap	54.87	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.487		Crippen Method
mcvol	217.760	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1192.00		NIST Webbook
tb	636.08	K	Joback Method
tc	804.10	K	Joback Method
tf	390.80	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.94	J/mol×K	636.08	Joback Method
cpg	630.77	J/mol×K	664.08	Joback Method
cpg	643.81	J/mol×K	692.09	Joback Method
cpg	656.09	J/mol×K	720.09	Joback Method
cpg	667.66	J/mol×K	748.09	Joback Method
cpg	678.53	J/mol×K	776.10	Joback Method
cpg	688.75	J/mol×K	804.10	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=U370838&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