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

Inchi: InChI=1S/C15H24F4O4/c1-4-7-8-9-22-12(20)14(5-2,6-3)13(21)23-10-15(18,19)11(16)17/
InchiKey: LZFYZFZDJRLBDF-UHFFFAOYSA-N
Formula: C15H24F4O4
SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 344.34

Physical Properties

Property code	Value	Unit	Source
gf	-1168.42	kJ/mol	Joback Method
hf	-1649.75	kJ/mol	Joback Method
hfus	34.15	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.970		Crippen Method
mcvol	244.170	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1476.00		NIST Webbook
rinpol	1476.00		NIST Webbook
tb	685.36	K	Joback Method
tc	855.20	K	Joback Method
tf	395.33	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.93	J/mol×K	685.36	Joback Method
cpg	728.94	J/mol×K	713.67	Joback Method
cpg	743.14	J/mol×K	741.97	Joback Method
cpg	756.55	J/mol×K	770.28	Joback Method
cpg	769.22	J/mol×K	798.59	Joback Method
cpg	781.15	J/mol×K	826.89	Joback Method
cpg	792.39	J/mol×K	855.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370833&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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