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

Inchi: InChI=1S/C17H29F3O4/c1-5-8-9-10-11-12-23-14(21)16(6-2,7-3)15(22)24-13(4)17(18,19)

InchiKey: JCZGOAUZRBUVAU-UHFFFAOYSA-N

Formula: C17H29F3O4

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

Mol. weight [g/mol]: 354.40

Physical Properties

Property code	Value	Unit	Source
gf	-956.77	kJ/mol	Joback Method
hf	-1494.92	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	66.32	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.800		Crippen Method
mcvol	270.580	ml/mol	McGowan Method
pc	1233.74	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	731.85	K	Joback Method
tc	907.60	K	Joback Method
tf	417.28	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.32	J/mol×K	731.85	Joback Method
cpg	834.54	J/mol×K	761.14	Joback Method
cpg	849.87	J/mol×K	790.43	Joback Method
cpg	864.32	J/mol×K	819.72	Joback Method
cpg	877.93	J/mol×K	849.01	Joback Method
cpg	890.74	J/mol×K	878.30	Joback Method
cpg	902.78	J/mol×K	907.60	Joback Method

Sources

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=U370819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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