Diethylmalonic acid, propyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C18H23F3O4/c1-4-11-24-15(22)17(5-2,6-3)16(23)25-12-13-7-9-14(10-8-13)18

InchiKey: GLBRVHXXQXKLQH-UHFFFAOYSA-N

Formula: C18H23F3O4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-843.13	kJ/mol	Joback Method
hf	-1285.22	kJ/mol	Joback Method
hfus	36.01	kJ/mol	Joback Method
hvap	71.87	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.508		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	1862.00		NIST Webbook
tb	786.83	K	Joback Method
tc	983.02	K	Joback Method
tf	482.49	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.21	J/mol×K	786.83	Joback Method
cpg	801.81	J/mol×K	819.53	Joback Method
cpg	815.40	J/mol×K	852.23	Joback Method
cpg	828.03	J/mol×K	884.92	Joback Method
cpg	839.75	J/mol×K	917.62	Joback Method
cpg	850.61	J/mol×K	950.32	Joback Method
cpg	860.67	J/mol×K	983.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368400&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