Diethylmalonic acid, pentyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C20H27F3O4/c1-4-7-8-13-26-17(24)19(5-2,6-3)18(25)27-14-15-9-11-16(12-10

InchiKey: VPXNFOJKZZZSJN-UHFFFAOYSA-N

Formula: C20H27F3O4

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

Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-826.29	kJ/mol	Joback Method
hf	-1326.50	kJ/mol	Joback Method
hfus	41.19	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.288		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2036.00		NIST Webbook
tb	832.59	K	Joback Method
tc	1029.58	K	Joback Method
tf	505.03	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.05	J/mol×K	832.59	Joback Method
cpg	917.16	J/mol×K	865.42	Joback Method
cpg	931.23	J/mol×K	898.25	Joback Method
cpg	944.30	J/mol×K	931.08	Joback Method
cpg	956.44	J/mol×K	963.92	Joback Method
cpg	967.70	J/mol×K	996.75	Joback Method
cpg	978.13	J/mol×K	1029.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368403&Units=SI

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