Diethylmalonic acid, butyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C19H25F3O4/c1-4-7-12-25-16(23)18(5-2,6-3)17(24)26-13-14-8-10-15(11-9-14

InchiKey: KRROYZMYKLBHTH-UHFFFAOYSA-N

Formula: C19H25F3O4

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

Mol. weight [g/mol]: 374.39

Physical Properties

Property code	Value	Unit	Source
gf	-834.71	kJ/mol	Joback Method
hf	-1305.86	kJ/mol	Joback Method
hfus	38.60	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.898		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	1945.00		NIST Webbook
tb	809.71	K	Joback Method
tc	1005.97	K	Joback Method
tf	493.76	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.20	J/mol×K	809.71	Joback Method
cpg	859.06	J/mol×K	842.42	Joback Method
cpg	872.89	J/mol×K	875.13	Joback Method
cpg	885.74	J/mol×K	907.84	Joback Method
cpg	897.68	J/mol×K	940.55	Joback Method
cpg	908.74	J/mol×K	973.26	Joback Method
cpg	918.99	J/mol×K	1005.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368402&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