Diethylmalonic acid, hexyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C21H29F3O4/c1-4-7-8-9-14-27-18(25)20(5-2,6-3)19(26)28-15-16-10-12-17(13

InchiKey: JGODUDZMZWRXBW-UHFFFAOYSA-N

Formula: C21H29F3O4

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

Mol. weight [g/mol]: 402.45

Physical Properties

Property code	Value	Unit	Source
gf	-817.87	kJ/mol	Joback Method
hf	-1347.14	kJ/mol	Joback Method
hfus	43.78	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.678		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2128.00		NIST Webbook
tb	855.47	K	Joback Method
tc	1053.89	K	Joback Method
tf	516.30	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.69	J/mol×K	855.47	Joback Method
cpg	976.07	J/mol×K	888.54	Joback Method
cpg	990.38	J/mol×K	921.61	Joback Method
cpg	1003.68	J/mol×K	954.68	Joback Method
cpg	1016.02	J/mol×K	987.75	Joback Method
cpg	1027.46	J/mol×K	1020.82	Joback Method
cpg	1038.07	J/mol×K	1053.89	Joback Method

Sources

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=U368404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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