Diethylmalonic acid, heptyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C22H31F3O4/c1-4-7-8-9-10-15-28-19(26)21(5-2,6-3)20(27)29-16-17-11-13-18

InchiKey: VVYGHTWDCYNTHE-UHFFFAOYSA-N

Formula: C22H31F3O4

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

Mol. weight [g/mol]: 416.47

Physical Properties

Property code	Value	Unit	Source
gf	-809.45	kJ/mol	Joback Method
hf	-1367.78	kJ/mol	Joback Method
hfus	46.37	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.069		Crippen Method
mcvol	317.270	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	2223.00		NIST Webbook
rinpol	2223.00		NIST Webbook
tb	878.35	K	Joback Method
tc	1078.97	K	Joback Method
tf	527.57	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.08	J/mol×K	878.35	Joback Method
cpg	1035.75	J/mol×K	911.79	Joback Method
cpg	1050.31	J/mol×K	945.22	Joback Method
cpg	1063.83	J/mol×K	978.66	Joback Method
cpg	1076.38	J/mol×K	1012.10	Joback Method
cpg	1088.02	J/mol×K	1045.54	Joback Method
cpg	1098.80	J/mol×K	1078.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368405&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

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