Diethylmalonic acid, di(4-trifluoromethylbenzyl) ester

Inchi: InChI=1S/C23H22F6O4/c1-3-21(4-2,19(30)32-13-15-5-9-17(10-6-15)22(24,25)26)20(31)
InchiKey: MCWGFITXDWIRIW-UHFFFAOYSA-N
Formula: C23H22F6O4
SMILES: CCC(CC)(C(=O)OCc1ccc(C(F)(F)F)cc1)C(=O)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 476.41

Physical Properties

Property code	Value	Unit	Source
gf	-1279.84	kJ/mol	Joback Method
hf	-1760.44	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.317		Crippen Method
mcvol	312.910	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	927.47	K	Joback Method
tc	1140.44	K	Joback Method
tf	581.97	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.90	J/mol×K	927.47	Joback Method
cpg	1012.54	J/mol×K	962.97	Joback Method
cpg	1024.17	J/mol×K	998.46	Joback Method
cpg	1034.91	J/mol×K	1033.96	Joback Method
cpg	1044.85	J/mol×K	1069.45	Joback Method
cpg	1054.11	J/mol×K	1104.95	Joback Method
cpg	1062.77	J/mol×K	1140.44	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=U368407&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