Diethylmalonic acid, octyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C23H33F3O4/c1-4-7-8-9-10-11-16-29-20(27)22(5-2,6-3)21(28)30-17-18-12-14

InchiKey: NQJFJIAOWFJGSJ-UHFFFAOYSA-N

Formula: C23H33F3O4

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

Mol. weight [g/mol]: 430.50

Physical Properties

Property code	Value	Unit	Source
gf	-801.03	kJ/mol	Joback Method
hf	-1388.42	kJ/mol	Joback Method
hfus	48.96	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.459		Crippen Method
mcvol	331.360	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	901.23	K	Joback Method
tc	1104.88	K	Joback Method
tf	538.84	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1080.16	J/mol×K	901.23	Joback Method
cpg	1096.13	J/mol×K	935.17	Joback Method
cpg	1110.97	J/mol×K	969.11	Joback Method
cpg	1124.74	J/mol×K	1003.05	Joback Method
cpg	1137.50	J/mol×K	1036.99	Joback Method
cpg	1149.34	J/mol×K	1070.94	Joback Method
cpg	1160.31	J/mol×K	1104.88	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=U368406&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

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