Malonic acid, (alpha,alpha,alpha-trifluoro-m-toluidine)methylene diethyl ester

Other names: diethyl [(«alpha»,«alpha»,«alpha»-trifluoro-m-toluidino)methylene]malonate
Inchi: InChI=1S/C15H16F3NO4/c1-3-22-13(20)12(14(21)23-4-2)9-19-11-7-5-6-10(8-11)15(16,1
InchiKey: RFRRNORICIZXCP-UHFFFAOYSA-N
Formula: C15H16F3NO4
SMILES: CCOC(=O)C(=CNc1cccc(C(F)(F)F)c1)C(=O)OCC
Mol. weight [g/mol]: 331.29
CAS: 370-35-4

Physical Properties

Property code	Value	Unit	Source
gf	-710.17	kJ/mol	Joback Method
hf	-1053.65	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	72.96	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.127		Crippen Method
mcvol	224.320	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
tb	775.63	K	Joback Method
tc	977.01	K	Joback Method
tf	479.88	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.13	J/mol×K	775.63	Joback Method
cpg	660.53	J/mol×K	809.19	Joback Method
cpg	672.04	J/mol×K	842.76	Joback Method
cpg	682.70	J/mol×K	876.32	Joback Method
cpg	692.56	J/mol×K	909.88	Joback Method
cpg	701.66	J/mol×K	943.44	Joback Method
cpg	710.03	J/mol×K	977.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C370354&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume