Diethylmalonic acid, ethyl 2-fluorophenyl ester

Inchi: InChI=1S/C15H19FO4/c1-4-15(5-2,13(17)19-6-3)14(18)20-12-10-8-7-9-11(12)16/h7-10H
InchiKey: YVMGEKAQQQHRCG-UHFFFAOYSA-N
Formula: C15H19FO4
SMILES: CCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F
Mol. weight [g/mol]: 282.31

Physical Properties

Property code	Value	Unit	Source
gf	-481.61	kJ/mol	Joback Method
hf	-822.33	kJ/mol	Joback Method
hfus	29.50	kJ/mol	Joback Method
hvap	68.12	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.101		Crippen Method
mcvol	215.100	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1725.00		NIST Webbook
tb	722.88	K	Joback Method
tc	928.08	K	Joback Method
tf	445.08	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.88	J/mol×K	722.88	Joback Method
cpg	618.42	J/mol×K	757.08	Joback Method
cpg	631.98	J/mol×K	791.28	Joback Method
cpg	644.59	J/mol×K	825.48	Joback Method
cpg	656.28	J/mol×K	859.68	Joback Method
cpg	667.08	J/mol×K	893.88	Joback Method
cpg	677.01	J/mol×K	928.08	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=U370125&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