diethyl formamidomalonate

Inchi: InChI=1S/C8H13NO5/c1-3-13-7(11)6(9-5-10)8(12)14-4-2/h5-6H,3-4H2,1-2H3,(H,9,10)
InchiKey: PFLHGSJLYNJIOF-UHFFFAOYSA-N
Formula: C8H13NO5
SMILES: CCOC(=O)C(NC=O)C(=O)OCC
Mol. weight [g/mol]: 203.19
CAS: 6326-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-463.93	kJ/mol	Joback Method
hf	-735.44	kJ/mol	Joback Method
hfus	25.91	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	-0.773		Crippen Method
mcvol	150.010	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
tb	633.41	K	Joback Method
tc	825.79	K	Joback Method
tf	325.00 ± 3.00	K	NIST Webbook
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.93	J/mol×K	633.41	Joback Method
cpg	396.74	J/mol×K	665.47	Joback Method
cpg	407.00	J/mol×K	697.54	Joback Method
cpg	416.70	J/mol×K	729.60	Joback Method
cpg	425.83	J/mol×K	761.67	Joback Method
cpg	434.40	J/mol×K	793.73	Joback Method
cpg	442.38	J/mol×K	825.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.70	K	1.50	NIST Webbook

Sources

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=C6326449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume