2-Dimethylaminomethylene-4-methyl-3-pentenoic acid, methyl ester

Inchi: InChI=1S/C10H17NO2/c1-8(2)6-9(7-11(3)4)10(12)13-5/h6-7H,1-5H3/b9-7+

InchiKey: XOQYXIZPLUWJHB-VQHVLOKHSA-N

Formula: C10H17NO2

SMILES: COC(=O)C(C=C(C)C)=CN(C)C

Mol. weight [g/mol]: 183.25

CAS: 90978-52-2

Physical Properties

Property code	Value	Unit	Source
gf	53.52	kJ/mol	Joback Method
hf	-212.14	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.571		Crippen Method
mcvol	160.580	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
tb	525.01	K	Joback Method
tc	717.16	K	Joback Method
tf	269.01	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.97	J/mol×K	525.01	Joback Method
cpg	381.49	J/mol×K	557.04	Joback Method
cpg	395.25	J/mol×K	589.06	Joback Method
cpg	408.27	J/mol×K	621.09	Joback Method
cpg	420.60	J/mol×K	653.11	Joback Method
cpg	432.26	J/mol×K	685.14	Joback Method
cpg	443.30	J/mol×K	717.16	Joback Method

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=C90978522&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume