3-Methylbut-2-enoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C11H20O3/c1-9(2)7-11(12)14-8-10(3)5-6-13-4/h7,10H,5-6,8H2,1-4H3

InchiKey: HUBXSBGOYZNBHQ-UHFFFAOYSA-N

Formula: C11H20O3

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

Mol. weight [g/mol]: 200.27

Physical Properties

Property code	Value	Unit	Source
gf	-227.95	kJ/mol	Joback Method
hf	-545.24	kJ/mol	Joback Method
hfus	23.59	kJ/mol	Joback Method
hvap	51.30	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.168		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1421.00		NIST Webbook
tb	553.39	K	Joback Method
tc	737.01	K	Joback Method
tf	274.08	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.80	J/mol×K	553.39	Joback Method
cpg	438.71	J/mol×K	583.99	Joback Method
cpg	452.99	J/mol×K	614.60	Joback Method
cpg	466.65	J/mol×K	645.20	Joback Method
cpg	479.70	J/mol×K	675.80	Joback Method
cpg	492.14	J/mol×K	706.41	Joback Method
cpg	503.99	J/mol×K	737.01	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=U355130&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