4-Methylpentan-2-yl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C11H20O2/c1-6-9(4)11(12)13-10(5)7-8(2)3/h6,8,10H,7H2,1-5H3/b9-6+
InchiKey: KIDWQYKYQAMOLE-RMKNXTFCSA-N
Formula: C11H20O2
SMILES: CC=C(C)C(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-125.39	kJ/mol	Joback Method
hf	-418.30	kJ/mol	Joback Method
hfus	18.88	kJ/mol	Joback Method
hvap	48.50	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.930		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1196.00		NIST Webbook
tb	530.53	K	Joback Method
tc	718.97	K	Joback Method
tf	236.85	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.70	J/mol×K	530.53	Joback Method
cpg	413.26	J/mol×K	561.94	Joback Method
cpg	428.11	J/mol×K	593.34	Joback Method
cpg	442.26	J/mol×K	624.75	Joback Method
cpg	455.74	J/mol×K	656.16	Joback Method
cpg	468.56	J/mol×K	687.56	Joback Method
cpg	480.74	J/mol×K	718.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373761&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume