2,4-Dimethylpentan-3-yl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C12H22O2/c1-7-10(6)12(13)14-11(8(2)3)9(4)5/h7-9,11H,1-6H3/b10-7+

InchiKey: FTLKZZLRHWGGDE-JXMROGBWSA-N

Formula: C12H22O2

SMILES: CC=C(C)C(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-119.41	kJ/mol	Joback Method
hf	-444.22	kJ/mol	Joback Method
hfus	17.95	kJ/mol	Joback Method
hvap	50.34	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.176		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1259.00		NIST Webbook
rinpol	1259.00		NIST Webbook
tb	552.97	K	Joback Method
tc	742.96	K	Joback Method
tf	233.12	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.42	J/mol×K	552.97	Joback Method
cpg	463.06	J/mol×K	584.63	Joback Method
cpg	478.91	J/mol×K	616.30	Joback Method
cpg	494.00	J/mol×K	647.96	Joback Method
cpg	508.35	J/mol×K	679.63	Joback Method
cpg	521.97	J/mol×K	711.29	Joback Method
cpg	534.90	J/mol×K	742.96	Joback Method

Sources

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=U373755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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