4-Hepten-2-ol, (Z)-, 3-methylbutanoate

Other names: (Z)-4-Hepten-2-yl 3-methylbutanoate
Inchi: InChI=1S/C12H22O2/c1-5-6-7-8-11(4)14-12(13)9-10(2)3/h6-7,10-11H,5,8-9H2,1-4H3/b7-
InchiKey: VFIBGALLMLBUTC-SREVYHEPSA-N
Formula: C12H22O2
SMILES: CCC=CCC(C)OC(=O)CC(C)C
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-108.42	kJ/mol	Joback Method
hf	-429.15	kJ/mol	Joback Method
hfus	22.78	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.320		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1246.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1248.00		NIST Webbook
tb	553.53	K	Joback Method
tc	736.79	K	Joback Method
tf	262.08	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.33	J/mol×K	553.53	Joback Method
cpg	462.35	J/mol×K	584.07	Joback Method
cpg	477.65	J/mol×K	614.62	Joback Method
cpg	492.24	J/mol×K	645.16	Joback Method
cpg	506.15	J/mol×K	675.70	Joback Method

cpg	519.39	J/mol×K	706.25	Joback Method
cpg	531.97	J/mol×K	736.79	Joback Method
dvisc	0.0059039	Pa×s	262.08	Joback Method
dvisc	0.0019456	Pa×s	310.66	Joback Method
dvisc	0.0008657	Pa×s	359.23	Joback Method
dvisc	0.0004671	Pa×s	407.81	Joback Method
dvisc	0.0002874	Pa×s	456.38	Joback Method
dvisc	0.0001942	Pa×s	504.95	Joback Method
dvisc	0.0001405	Pa×s	553.53	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=R75610&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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