Heptyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C12H22O2/c1-4-6-7-8-9-10-14-12(13)11(3)5-2/h5H,4,6-10H2,1-3H3/b11-5+
InchiKey: AHFSPERSNRDCGH-VZUCSPMQSA-N
Formula: C12H22O2
SMILES: CC=C(C)C(=O)OCCCCCCC
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-112.09	kJ/mol	Joback Method
hf	-428.38	kJ/mol	Joback Method
hfus	28.52	kJ/mol	Joback Method
hvap	51.50	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1429.00		NIST Webbook
rinpol	1429.00		NIST Webbook
tb	554.29	K	Joback Method
tc	733.58	K	Joback Method
tf	278.12	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.54	J/mol×K	554.29	Joback Method
cpg	461.07	J/mol×K	584.17	Joback Method
cpg	475.92	J/mol×K	614.05	Joback Method
cpg	490.12	J/mol×K	643.93	Joback Method
cpg	503.67	J/mol×K	673.81	Joback Method
cpg	516.59	J/mol×K	703.70	Joback Method
cpg	528.92	J/mol×K	733.58	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=U373738&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