(Z)-Non-3-enyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C14H24O2/c1-4-6-7-8-9-10-11-12-16-14(15)13(3)5-2/h5,9-10H,4,6-8,11-12H2,
InchiKey: PHYVRJBNPCQLHO-RBUNJRTFSA-N
Formula: C14H24O2
SMILES: CC=C(C)C(=O)OCCC=CCCCCC
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-15.03	kJ/mol	Joback Method
hf	-352.44	kJ/mol	Joback Method
hfus	33.90	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.022		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1612.00		NIST Webbook
rinpol	1612.00		NIST Webbook
tb	604.21	K	Joback Method
tc	787.04	K	Joback Method
tf	295.58	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.38	J/mol×K	604.21	Joback Method
cpg	543.69	J/mol×K	634.68	Joback Method
cpg	559.23	J/mol×K	665.15	Joback Method
cpg	574.01	J/mol×K	695.62	Joback Method
cpg	588.08	J/mol×K	726.10	Joback Method
cpg	601.47	J/mol×K	756.57	Joback Method
cpg	614.21	J/mol×K	787.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373731&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