Nonyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C14H26O2/c1-4-6-7-8-9-10-11-12-16-14(15)13(3)5-2/h5H,4,6-12H2,1-3H3/b13
InchiKey: NIOMGUSCYSQFTC-WLRTZDKTSA-N
Formula: C14H26O2
SMILES: CC=C(C)C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 226.35

Physical Properties

Property code	Value	Unit	Source
gf	-95.25	kJ/mol	Joback Method
hf	-469.66	kJ/mol	Joback Method
hfus	33.70	kJ/mol	Joback Method
hvap	55.95	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.246		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	1628.00		NIST Webbook
tb	600.05	K	Joback Method
tc	776.39	K	Joback Method
tf	300.66	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.21	J/mol×K	600.05	Joback Method
cpg	563.92	J/mol×K	629.44	Joback Method
cpg	579.89	J/mol×K	658.83	Joback Method
cpg	595.14	J/mol×K	688.22	Joback Method
cpg	609.70	J/mol×K	717.61	Joback Method
cpg	623.58	J/mol×K	747.00	Joback Method
cpg	636.81	J/mol×K	776.39	Joback Method

Sources

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=U373746&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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