4-Methylpentyl 8-methylnon-6-enoate

Inchi: InChI=1S/C16H30O2/c1-14(2)10-7-5-6-8-12-16(17)18-13-9-11-15(3)4/h7,10,14-15H,5-6,
InchiKey: OVYHDLFPFWJOMW-JXMROGBWSA-N
Formula: C16H30O2
SMILES: CC(C)C=CCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 254.41
CAS: 1215128-18-9

Physical Properties

Property code	Value	Unit	Source
gf	-74.74	kJ/mol	Joback Method
hf	-511.71	kJ/mol	Joback Method
hfus	33.14	kJ/mol	Joback Method
hvap	59.55	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.738		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	1692.20		NIST Webbook
rinpol	1692.20		NIST Webbook
tb	645.05	K	Joback Method
tc	822.49	K	Joback Method
tf	307.16	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.91	J/mol×K	645.05	Joback Method
cpg	673.97	J/mol×K	674.62	Joback Method
cpg	691.19	J/mol×K	704.20	Joback Method
cpg	707.60	J/mol×K	733.77	Joback Method
cpg	723.22	J/mol×K	763.35	Joback Method
cpg	738.07	J/mol×K	792.92	Joback Method
cpg	752.19	J/mol×K	822.49	Joback Method

dvisc	0.0041086	Pa×s	307.16	Joback Method
dvisc	0.0013293	Pa×s	363.48	Joback Method
dvisc	0.0005821	Pa×s	419.79	Joback Method
dvisc	0.0003099	Pa×s	476.11	Joback Method
dvisc	0.0001885	Pa×s	532.42	Joback Method
dvisc	0.0001261	Pa×s	588.73	Joback Method
dvisc	0.0000905	Pa×s	645.05	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=C1215128189&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
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

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