

4-Methylpentyl 8-methylnonanoate

Inchi:	InChI=1S/C16H32O2/c1-14(2)10-7-5-6-8-12-16(17)18-13-9-11-15(3)4/h14-15H,5-13H2,1
InchiKey:	DZMWJKCEEYZSQX-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CC(C)CCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	256.42
CAS:	1215127-97-1

Physical Properties

Property code	Value	Unit	Source
gf	-154.96	kJ/mol	Joback Method
hf	-628.93	kJ/mol	Joback Method
hfus	32.94	kJ/mol	Joback Method
hvap	59.59	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.962		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	1710.10		NIST Webbook
rinpol	1710.10		NIST Webbook
tb	640.89	K	Joback Method
tc	812.85	K	Joback Method
tf	312.24	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.61	J/molxK	640.89	Joback Method
cpg	760.94	J/molxK	784.19	Joback Method
cpg	745.63	J/molxK	755.53	Joback Method
cpg	729.56	J/molxK	726.87	Joback Method
cpg	712.71	J/molxK	698.21	Joback Method
cpg	695.06	J/molxK	669.55	Joback Method
cpg	775.50	J/molxK	812.85	Joback Method

dvisc	0.0001055	Paxs	640.89	Joback Method
dvisc	0.0001468	Paxs	586.12	Joback Method
dvisc	0.0002184	Paxs	531.34	Joback Method
dvisc	0.0003562	Paxs	476.56	Joback Method
dvisc	0.0006596	Paxs	421.79	Joback Method
dvisc	0.0014680	Paxs	367.01	Joback Method
dvisc	0.0043257	Paxs	312.24	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=C1215127971&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

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