

Isobutyl 8-methylnon-6-enoate

Inchi:	InChI=1S/C14H26O2/c1-12(2)9-7-5-6-8-10-14(15)16-11-13(3)4/h7,9,12-13H,5-6,8,10-11H
InchiKey:	QRIKILMASWEEMP-VQHVLOKHSA-N
Formula:	C14H26O2
SMILES:	CC(C)C=CCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	226.35
CAS:	1215128-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-91.58	kJ/mol	Joback Method
hf	-470.43	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	55.10	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.958		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	1496.40		NIST Webbook
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tb	599.29	K	Joback Method
tc	779.11	K	Joback Method
tf	284.62	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.16	J/molxK	599.29	Joback Method
cpg	626.35	J/molxK	749.14	Joback Method
cpg	612.19	J/molxK	719.17	Joback Method
cpg	597.32	J/molxK	689.20	Joback Method
cpg	581.71	J/molxK	659.23	Joback Method
cpg	565.33	J/molxK	629.26	Joback Method
cpg	639.81	J/molxK	779.11	Joback Method

dvisc	0.0001141	Paxs	599.29	Joback Method
dvisc	0.0001584	Paxs	546.85	Joback Method
dvisc	0.0002357	Paxs	494.40	Joback Method
dvisc	0.0003855	Paxs	441.95	Joback Method
dvisc	0.0007196	Paxs	389.51	Joback Method
dvisc	0.0016313	Paxs	337.06	Joback Method
dvisc	0.0049998	Paxs	284.62	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=C1215128156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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