

isobutyl 9-decenoate

Inchi:	InChI=1S/C14H26O2/c1-4-5-6-7-8-9-10-11-14(15)16-12-13(2)3/h4,13H,1,5-12H2,2-3H3
InchiKey:	LVTDNTADTOUODR-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	C=CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	226.35

Physical Properties

Property code	Value	Unit	Source
gf	-81.52	kJ/mol	Joback Method
hf	-456.94	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	54.86	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.102		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
ripol	1788.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1788.00		NIST Webbook
tb	592.25	K	Joback Method
tc	765.51	K	Joback Method
tf	302.94	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.03	J/molxK	592.25	Joback Method
cpg	562.74	J/molxK	621.13	Joback Method
cpg	578.74	J/molxK	650.00	Joback Method
cpg	594.03	J/molxK	678.88	Joback Method
cpg	608.62	J/molxK	707.76	Joback Method

cpg	622.55	J/mol×K	736.63	Joback Method
cpg	635.82	J/mol×K	765.51	Joback Method
dvisc	0.0035593	Paxs	302.94	Joback Method
dvisc	0.0014576	Paxs	351.16	Joback Method
dvisc	0.0007405	Paxs	399.38	Joback Method
dvisc	0.0004353	Paxs	447.60	Joback Method
dvisc	0.0002838	Paxs	495.81	Joback Method
dvisc	0.0001995	Paxs	544.03	Joback Method
dvisc	0.0001486	Paxs	592.25	Joback Method

Sources

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=R313718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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