Isobutyl 10-undecenoate

Other names: isobutyl undec-10-enoate
Inchi: InChI=1S/C15H28O2/c1-4-5-6-7-8-9-10-11-12-15(16)17-13-14(2)3/h4,14H,1,5-13H2,2-3H
InchiKey: YXJSBTYPYXKWDB-UHFFFAOYSA-N
Formula: C15H28O2
SMILES: C=CCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 240.38
CAS: 5421-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-73.10	kJ/mol	Joback Method
hf	-477.58	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	57.08	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.492		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1900.00		NIST Webbook
tb	615.13	K	Joback Method
tc	787.46	K	Joback Method
tf	314.21	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.05	J/mol×K	615.13	Joback Method
cpg	616.27	J/mol×K	643.85	Joback Method
cpg	632.74	J/mol×K	672.57	Joback Method
cpg	648.48	J/mol×K	701.29	Joback Method

cpg	663.50	J/mol×K	730.01	Joback Method
cpg	677.81	J/mol×K	758.74	Joback Method
cpg	691.45	J/mol×K	787.46	Joback Method
dvisc	0.0033107	Pa×s	314.21	Joback Method
dvisc	0.0013405	Pa×s	364.36	Joback Method
dvisc	0.0006755	Pa×s	414.52	Joback Method
dvisc	0.0003947	Pa×s	464.67	Joback Method
dvisc	0.0002561	Pa×s	514.82	Joback Method
dvisc	0.0001794	Pa×s	564.98	Joback Method
dvisc	0.0001332	Pa×s	615.13	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5421272&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume