

2-(2-Isopentoxyethoxy)ethyl acetate

Inchi:	InChI=1S/C11H22O4/c1-10(2)4-5-13-6-7-14-8-9-15-11(3)12/h10H,4-9H2,1-3H3
InchiKey:	BAHUAGUWSSWQFO-UHFFFAOYSA-N
Formula:	C11H22O4
SMILES:	CC(=O)OCCOCCOCCC(C)C
Mol. weight [g/mol]:	218.29

Physical Properties

Property code	Value	Unit	Source
gf	-404.62	kJ/mol	Joback Method
hf	-784.89	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.629		Crippen Method
mcvol	185.030	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1463.50		NIST Webbook
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tb	571.77	K	Joback Method
tc	744.96	K	Joback Method
tf	315.35	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.67	J/molxK	571.77	Joback Method
cpg	484.57	J/molxK	600.63	Joback Method
cpg	498.93	J/molxK	629.50	Joback Method
cpg	512.74	J/molxK	658.36	Joback Method
cpg	526.00	J/molxK	687.23	Joback Method
cpg	538.69	J/molxK	716.09	Joback Method
cpg	550.81	J/molxK	744.96	Joback Method
dvisc	0.0021183	Paxs	315.35	Joback Method

dvisc	0.0009950	Paxs	358.09	Joback Method
dvisc	0.0005491	Paxs	400.82	Joback Method
dvisc	0.0003398	Paxs	443.56	Joback Method
dvisc	0.0002288	Paxs	486.30	Joback Method
dvisc	0.0001642	Paxs	529.03	Joback Method
dvisc	0.0001239	Paxs	571.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R188740&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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