

2-[2-(2-Isopentoxyethoxy)ethoxy]ethyl acetate

Inchi:	InChI=1S/C13H26O5/c1-12(2)4-5-15-6-7-16-8-9-17-10-11-18-13(3)14/h12H,4-11H2,1-3H
InchiKey:	NEJMUHOSTHFGMW-UHFFFAOYSA-N
Formula:	C13H26O5
SMILES:	CC(=O)OCCOCCOCCOCCC(C)C
Mol. weight [g/mol]:	262.34

Physical Properties

Property code	Value	Unit	Source
gf	-492.78	kJ/mol	Joback Method
hf	-958.39	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	60.53	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	1.645		Crippen Method
mcvol	219.080	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	1746.70		NIST Webbook
rinpol	1746.70		NIST Webbook
tb	639.95	K	Joback Method
tc	811.31	K	Joback Method
tf	360.12	K	Joback Method
vc	0.836	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.60	J/molxK	639.95	Joback Method
cpg	617.64	J/molxK	668.51	Joback Method
cpg	633.03	J/molxK	697.07	Joback Method
cpg	647.77	J/molxK	725.63	Joback Method
cpg	661.84	J/molxK	754.19	Joback Method
cpg	675.23	J/molxK	782.75	Joback Method
cpg	687.92	J/molxK	811.31	Joback Method
dvisc	0.0012527	Paxs	360.12	Joback Method

dvisc	0.0006010	Paxs	406.76	Joback Method
dvisc	0.0003354	Paxs	453.40	Joback Method
dvisc	0.0002086	Paxs	500.04	Joback Method
dvisc	0.0001408	Paxs	546.67	Joback Method
dvisc	0.0001010	Paxs	593.31	Joback Method
dvisc	0.0000761	Paxs	639.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188577&Units=SI
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

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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