

2-(2-(2-(2-(2-(2-Isopentoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxy

Inchi:
acetate

InChI=1S/C21H42O9/c1-20(2)4-5-23-6-7-24-8-9-25-10-11-26-12-13-27-14-15-28-16-17-2

InchiKey:

UZDYGKHEJAATER-UHFFFAOYSA-N

Formula:

C21H42O9

SMILES:

CC(=O)OCCOCCOCCOCCOCCOCCOCCOCCOCC(C)C

Mol. weight [g/mol]:

438.55

Physical Properties

Property code	Value	Unit	Source
gf	-845.42	kJ/mol	Joback Method
hf	-1652.39	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	87.98	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	1.712		Crippen Method
mcvol	355.280	ml/mol	McGowan Method
pc	918.83	kPa	Joback Method
rinpol	2874.60		NIST Webbook
rinpol	2874.60		NIST Webbook
tb	912.67	K	Joback Method
tc	1120.93	K	Joback Method
tf	539.20	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1197.92	J/molxK	912.67	Joback Method
cpg	1269.53	J/molxK	1086.22	Joback Method
cpg	1259.32	J/molxK	1051.51	Joback Method
cpg	1247.00	J/molxK	1016.80	Joback Method
cpg	1232.63	J/molxK	982.09	Joback Method
cpg	1216.25	J/molxK	947.38	Joback Method
cpg	1277.57	J/molxK	1120.93	Joback Method
dvisc	0.0000073	Paxs	912.67	Joback Method

dvisc	0.0000098	Paxs	850.43	Joback Method
dvisc	0.0000136	Paxs	788.18	Joback Method
dvisc	0.0000199	Paxs	725.94	Joback Method
dvisc	0.0000316	Paxs	663.69	Joback Method
dvisc	0.0000549	Paxs	601.45	Joback Method
dvisc	0.0001084	Paxs	539.20	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=R187990&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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