

2-(2-(2-(2-(2-(2-(2-Isobutoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxy)acetate

InChI: InChI=1S/C22H44O10/c1-21(2)20-31-17-16-29-13-12-27-9-8-25-5-4-24-6-7-26-10-11-28
InChIKey: JBMAVCLRPVPEGL-UHFFFAOYSA-N
Formula: C22H44O10
SMILES: CC(=O)OCCOCCOCCOCCOCCOCCOCCOCCOCC(C)C
Mol. weight [g/mol]: 468.58

Physical Properties

Property code	Value	Unit	Source
gf	-942.00	kJ/mol	Joback Method
hf	-1805.25	kJ/mol	Joback Method
hfus	61.50	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	1.338		Crippen Method
mcvol	375.240	ml/mol	McGowan Method
pc	858.98	kPa	Joback Method
rinpol	3060.60		NIST Webbook
rinpol	3060.60		NIST Webbook
tb	957.97	K	Joback Method
tc	1183.72	K	Joback Method
tf	572.70	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1290.74	J/mol×K	957.97	Joback Method
cpg	1308.48	J/mol×K	995.59	Joback Method
cpg	1323.64	J/mol×K	1033.22	Joback Method
cpg	1336.14	J/mol×K	1070.84	Joback Method
cpg	1345.89	J/mol×K	1108.47	Joback Method
cpg	1352.83	J/mol×K	1146.09	Joback Method
cpg	1356.86	J/mol×K	1183.72	Joback Method
dvisc	0.0000641	Pa×s	572.70	Joback Method

dvisc	0.0000330	Pa×s	636.91	Joback Method
dvisc	0.0000192	Pa×s	701.12	Joback Method
dvisc	0.0000122	Pa×s	765.34	Joback Method
dvisc	0.0000084	Pa×s	829.55	Joback Method
dvisc	0.0000060	Pa×s	893.76	Joback Method
dvisc	0.0000046	Pa×s	957.97	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R187816&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

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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