2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Acetyloxyethoxy acetate

Other names: Tridecaethylene glycol, diacetate

40-Oxo-3,6,9,12,15,18,21,24,27,30,33,36,39-tridecaoxahentetracont-1-yl acetate

Inchi: InChI=1S/C30H58O16/c1-29(31)45-27-25-43-23-21-41-19-17-39-15-13-37-11-9-35-7-5-3

InchiKey: UJHRMHHOVCLYEK-UHFFFAOYSA-N

Formula: C30H58O16

SMILES: CC(=O)OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOC(C)=O

Mol. weight [g/mol]: 674.77

Physical Properties

Property code	Value	Unit	Source
gf	-1526.12	kJ/mol	Joback Method
hf	-2738.77	kJ/mol	Joback Method
hfus	93.29	kJ/mol	Joback Method
hvap	129.61	kJ/mol	Joback Method
log10ws	0.85		Crippen Method
logp	0.312		Crippen Method
mcvol	518.880	ml/mol	McGowan Method
pc	564.20	kPa	Joback Method
rinpol	4354.90		NIST Webbook
rinpol	4354.90		NIST Webbook
tb	1307.42	K	Joback Method
tc	1879.85	K	Joback Method
tf	838.94	K	Joback Method
vc	1.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1837.60	J/mol×K	1307.42	Joback Method
cpg	1784.69	J/mol×K	1402.82	Joback Method
cpg	1697.80	J/mol×K	1498.23	Joback Method
cpg	1574.65	J/mol×K	1593.63	Joback Method
cpg	1412.94	J/mol×K	1689.04	Joback Method
cpg	1210.39	J/mol×K	1784.44	Joback Method

cpg	964.71	J/mol×K	1879.85	Joback Method
dvisc	0.0000022	Pa×s	838.94	Joback Method
dvisc	0.0000013	Pa×s	917.02	Joback Method
dvisc	0.0000008	Pa×s	995.10	Joback Method
dvisc	0.0000005	Pa×s	1073.18	Joback Method
dvisc	0.0000004	Pa×s	1151.26	Joback Method
dvisc	0.0000003	Pa×s	1229.34	Joback Method
dvisc	0.0000002	Pa×s	1307.42	Joback Method

Sources

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=U351894&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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