

Octapropylene glycol, monoallyl ether, acetate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C29H56O10/c1-11-12-31-13-21(2)32-14-22(3)33-15-23(4)34-16-24(5)35-17-25

INQRCQNMYZGEB-UHFFFAOYSA-N

C29H56O10

C=CCOCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OC(C)=O

564.75

Physical Properties

Property code	Value	Unit	Source
gf	-812.30	kJ/mol	Joback Method
hf	-1861.26	kJ/mol	Joback Method
hfus	53.69	kJ/mol	Joback Method
hvap	104.81	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.976		Crippen Method
mcvol	469.570	ml/mol	McGowan Method
pc	629.40	kPa	Joback Method
rinpol	2916.00		NIST Webbook
rinpol	2911.00		NIST Webbook
rinpol	2914.00		NIST Webbook
rinpol	2911.00		NIST Webbook
rinpol	2914.00		NIST Webbook
rinpol	2916.00		NIST Webbook
rinpol	2916.00		NIST Webbook
rinpol	2911.00		NIST Webbook
rinpol	2914.00		NIST Webbook
rinpol	2916.00		NIST Webbook
rinpol	2911.00		NIST Webbook
rinpol	2912.00		NIST Webbook
rinpol	2914.00		NIST Webbook
rinpol	2916.00		NIST Webbook
rinpol	2912.00		NIST Webbook
tb	1111.73	K	Joback Method
tc	1404.60	K	Joback Method
tf	544.83	K	Joback Method
vc	1.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1695.51	J/mol×K	1111.73	Joback Method
cpg	1704.55	J/mol×K	1355.79	Joback Method
cpg	1713.89	J/mol×K	1306.98	Joback Method
cpg	1717.54	J/mol×K	1258.16	Joback Method
cpg	1715.63	J/mol×K	1209.35	Joback Method
cpg	1708.25	J/mol×K	1160.54	Joback Method
cpg	1689.42	J/mol×K	1404.60	Joback Method
dvisc	0.0000008	Pa×s	1111.73	Joback Method
dvisc	0.0000011	Pa×s	1017.25	Joback Method
dvisc	0.0000018	Pa×s	922.76	Joback Method
dvisc	0.0000032	Pa×s	828.28	Joback Method
dvisc	0.0000066	Pa×s	733.80	Joback Method
dvisc	0.0000166	Pa×s	639.31	Joback Method
dvisc	0.0000583	Pa×s	544.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R152226&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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