

Pentapropylene glycol, monoallyl ether, acetate

Inchi:	InChI=1S/C20H38O7/c1-8-9-22-10-15(2)23-11-16(3)24-12-17(4)25-13-18(5)26-14-19(6)2
InchiKey:	JJTCCLQKXCXQLOF-UHFFFAOYSA-N
Formula:	C20H38O7
SMILES:	C=CCOCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OC(C)=O
Mol. weight [g/mol]:	390.51

Physical Properties

Property code	Value	Unit	Source
gf	-565.76	kJ/mol	Joback Method
hf	-1263.00	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	78.71	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.761		Crippen Method
mcvol	325.150	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2127.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2126.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	839.87	K	Joback Method
tc	1030.20	K	Joback Method
tf	421.71	K	Joback Method
vc	1.220	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.61	J/molxK	839.87	Joback Method
cpg	1064.97	J/molxK	871.59	Joback Method
cpg	1081.99	J/molxK	903.31	Joback Method
cpg	1097.64	J/molxK	935.04	Joback Method
cpg	1111.90	J/molxK	966.76	Joback Method
cpg	1124.77	J/molxK	998.48	Joback Method
cpg	1136.21	J/molxK	1030.20	Joback Method
dvisc	0.0005885	Paxs	421.71	Joback Method
dvisc	0.0001942	Paxs	491.40	Joback Method
dvisc	0.0000844	Paxs	561.10	Joback Method
dvisc	0.0000441	Paxs	630.79	Joback Method
dvisc	0.0000262	Paxs	700.48	Joback Method
dvisc	0.0000171	Paxs	770.18	Joback Method
dvisc	0.0000120	Paxs	839.87	Joback Method

Sources

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=R152246&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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