

Heptaethylene glycol, butyl ether, acetate

Other names:2-(2-(2-(2-(2-(2-Butoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethyl acetate

Inchi:InChI=1S/C20H40O9/c1-3-4-5-22-6-7-23-8-9-24-10-11-25-12-13-26-14-15-27-16-17-28-19

InchiKey:TZCDZUAVPBRTCB-UHFFFAOYSA-N

Formula:C20H40O9

SMILES:CCCCOCCOCCOCCOCCOCCOCCOCCOCCOC(C)=O

Mol. weight [g/mol]:424.53

Physical Properties

Property code	Value	Unit	Source
gf	-851.40	kJ/mol	Joback Method
hf	-1626.47	kJ/mol	Joback Method
hfus	58.66	kJ/mol	Joback Method
hvap	86.14	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	1.466		Crippen Method
mcvol	341.190	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	2816.60		NIST Webbook
tb	890.23	K	Joback Method
tc	1091.97	K	Joback Method
tf	542.93	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1135.41	J/mol×K	890.23	Joback Method
cpg	1208.28	J/mol×K	1058.34	Joback Method
cpg	1197.39	J/mol×K	1024.72	Joback Method
cpg	1184.60	J/mol×K	991.10	Joback Method
cpg	1169.98	J/mol×K	957.48	Joback Method
cpg	1153.56	J/mol×K	923.85	Joback Method
cpg	1217.24	J/mol×K	1091.97	Joback Method
dvisc	0.0000094	Pa×s	890.23	Joback Method

dvisc	0.0000123	Pa×s	832.35	Joback Method
dvisc	0.0000167	Pa×s	774.46	Joback Method
dvisc	0.0000239	Pa×s	716.58	Joback Method
dvisc	0.0000363	Pa×s	658.70	Joback Method
dvisc	0.0000599	Pa×s	600.81	Joback Method
dvisc	0.0001098	Pa×s	542.93	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=R187910&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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