

Diglycolic acid, butyl octyl ester

Inchi:	InChI=1S/C16H30O5/c1-3-5-7-8-9-10-12-21-16(18)14-19-13-15(17)20-11-6-4-2/h3-14H2
InchiKey:	QJQIERZVGLTQFG-UHFFFAOYSA-N
Formula:	C16H30O5
SMILES:	CCCCCCCCOC(=O)COCC(=O)OCCCC
Mol. weight [g/mol]:	302.41

Physical Properties

Property code	Value	Unit	Source
gf	-489.00	kJ/mol	Joback Method
hf	-995.39	kJ/mol	Joback Method
hfus	43.96	kJ/mol	Joback Method
hvap	71.93	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.250		Crippen Method
mvol	257.050	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	740.48	K	Joback Method
tc	918.04	K	Joback Method
tf	436.63	K	Joback Method
vc	0.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.64	J/molxK	740.48	Joback Method
cpg	780.01	J/molxK	770.07	Joback Method
cpg	795.54	J/molxK	799.67	Joback Method
cpg	810.22	J/molxK	829.26	Joback Method
cpg	824.05	J/molxK	858.86	Joback Method
cpg	837.03	J/molxK	888.45	Joback Method
cpg	849.16	J/molxK	918.04	Joback Method
dvisc	0.0008707	Paxs	436.63	Joback Method

dvisc	0.0004605	Paxs	487.27	Joback Method
dvisc	0.0002746	Paxs	537.91	Joback Method
dvisc	0.0001790	Paxs	588.56	Joback Method
dvisc	0.0001249	Paxs	639.20	Joback Method
dvisc	0.0000918	Paxs	689.84	Joback Method
dvisc	0.0000704	Paxs	740.48	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=U382111&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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