

Butyl everninate

Inchi:	InChI=1S/C13H18O4/c1-4-5-6-17-13(15)12-9(2)7-10(16-3)8-11(12)14/h7-8,14H,4-6H2,1
InchiKey:	ZSVOVTULAAEJFS-UHFFFAOYSA-N
Formula:	C13H18O4
SMILES:	CCCCOC(=O)c1c(C)cc(OC)cc1O
Mol. weight [g/mol]:	238.28

Physical Properties

Property code	Value	Unit	Source
gf	-341.81	kJ/mol	Joback Method
hf	-652.39	kJ/mol	Joback Method
hfus	32.45	kJ/mol	Joback Method
hvap	72.71	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.666		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1878.30		NIST Webbook
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tb	712.81	K	Joback Method
tc	924.67	K	Joback Method
tf	493.84	K	Joback Method
vc	0.663	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.84	J/molxK	712.81	Joback Method
cpg	536.41	J/molxK	748.12	Joback Method
cpg	549.23	J/molxK	783.43	Joback Method
cpg	561.36	J/molxK	818.74	Joback Method
cpg	572.81	J/molxK	854.05	Joback Method
cpg	583.64	J/molxK	889.36	Joback Method
cpg	593.86	J/molxK	924.67	Joback Method
dvisc	0.0001794	Paxs	493.84	Joback Method

dvisc	0.0000962	Paxs	530.34	Joback Method
dvisc	0.0000559	Paxs	566.83	Joback Method
dvisc	0.0000347	Paxs	603.33	Joback Method
dvisc	0.0000228	Paxs	639.82	Joback Method
dvisc	0.0000156	Paxs	676.31	Joback Method
dvisc	0.0000111	Paxs	712.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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