

Ethyl p-bis(2-hydroxyethyl)aminobenzoate

Other names:

Benzoic acid, p-(bis(2-hydroxyethyl)amino)-, ethyl ester
Benzoic acid, 4-(bis(2-hydroxyethyl)amino)-, ethyl ester
PEG-25 PABA
Uvinul P 25

Inchi:

InChI=1S/C13H19NO4/c1-2-18-13(17)11-3-5-12(6-4-11)14(7-9-15)8-10-16/h3-6,15-16H,

InchiKey:

XFPHFLGZXKHBMU-UHFFFAOYSA-N

Formula:

C13H19NO4

SMILES:

CCOC(=O)c1ccc(N(CCO)CCO)cc1

Mol. weight [g/mol]:

253.29

CAS:

15716-30-0

Physical Properties

Property code	Value	Unit	Source
gf	-235.42	kJ/mol	Joback Method
hf	-568.32	kJ/mol	Joback Method
hfus	37.06	kJ/mol	Joback Method
hvap	92.03	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.654		Crippen Method
mcvol	199.430	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	801.59	K	Joback Method
tc	991.78	K	Joback Method
tf	501.48	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.55	J/molxK	801.59	Joback Method
cpg	604.52	J/molxK	833.29	Joback Method
cpg	614.80	J/molxK	864.99	Joback Method
cpg	624.40	J/molxK	896.69	Joback Method
cpg	633.35	J/molxK	928.39	Joback Method

cpg	641.69	J/mol×K	960.08	Joback Method
cpg	649.42	J/mol×K	991.78	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=C15716300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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