

Butetamate

Other names:

Benzeneacetic acid, «alpha»-ethyl-, 2-(diethylamino)ethyl ester
Butethamate
2-(Diethylamino)ethyl 2-phenylbutyrate
HH-105

Inchi:

InChI=1S/C16H25NO2/c1-4-15(14-10-8-7-9-11-14)16(18)19-13-12-17(5-2)6-3/h7-11,15H

InchiKey:

CKWHSYRZDLWQFV-UHFFFAOYSA-N

Formula:

C16H25NO2

SMILES:

CCC(C(=O)OCCN(CC)CC)c1ccccc1

Mol. weight [g/mol]:

263.38

CAS:

14007-64-8

Physical Properties

Property code	Value	Unit	Source
gf	70.67	kJ/mol	Joback Method
hf	-319.59	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	64.30	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.065		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	1754.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1754.00		NIST Webbook
tb	680.45	K	Joback Method
tc	877.00	K	Joback Method
tf	386.13	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.42	J/mol×K	680.45	Joback Method
cpg	658.06	J/mol×K	713.21	Joback Method
cpg	674.67	J/mol×K	745.97	Joback Method
cpg	690.27	J/mol×K	778.73	Joback Method
cpg	704.92	J/mol×K	811.49	Joback Method
cpg	718.63	J/mol×K	844.24	Joback Method
cpg	731.46	J/mol×K	877.00	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=C14007648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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