2-Butanol, 1-(dimethylamino)-2-methyl-, benzoate

Other names: Amyleine
Amylocaine
Stovaine
Stovine
1-[(dimethylamino)methyl]-1-methylpropyl benzoate

Inchi: InChI=1S/C14H21NO2/c1-5-14(2,11-15(3)4)17-13(16)12-9-7-6-8-10-12/h6-10H,5,11H2,1

InchiKey: FDMBBCOBEAVDAO-UHFFFAOYSA-N

Formula: C14H21NO2

SMILES: CCC(C)(CN(C)C)OC(=O)c1ccccc1

Mol. weight [g/mol]: 235.32

CAS: 644-26-8

Physical Properties

Property code	Value	Unit	Source
gf	59.11	kJ/mol	Joback Method
hf	-281.78	kJ/mol	Joback Method
hfus	24.45	kJ/mol	Joback Method
hvap	58.94	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.574		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1574.00		NIST Webbook
ripol	2029.00		NIST Webbook
tb	631.90	K	Joback Method
tc	840.31	K	Joback Method
tf	381.01	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.41	J/mol×K	631.90	Joback Method
cpg	552.79	J/mol×K	666.63	Joback Method
cpg	569.04	J/mol×K	701.37	Joback Method
cpg	584.20	J/mol×K	736.10	Joback Method
cpg	598.34	J/mol×K	770.84	Joback Method
cpg	611.52	J/mol×K	805.57	Joback Method
cpg	623.78	J/mol×K	840.31	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=C644268&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume