

Parbenate

Other names:	Benzoic acid, 4-(dimethylamino)-, ethyl ester Benzoic acid, p-(dimethylamino)-, ethyl ester Ethyl p-dimethylaminobenzoate Ethyl 4-(dimethylamino)benzoate N,N-Dimethylbenzocaine Ethyl-4-(N,N-dimethylamino)benzoate Quantacure EPD p-Dimethylaminobenzoic acid ethyl ester Speedcure EDB Kayacure EPA Quantacure EPD (Ethyl 4-dimethylamino benzoate)
Inchi:	InChI=1S/C11H15NO2/c1-4-14-11(13)9-5-7-10(8-6-9)12(2)3/h5-8H,4H2,1-3H3
InchiKey:	FZUGPQWGEGAKET-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CCOC(=O)c1ccc(N(C)C)cc1
Mol. weight [g/mol]:	193.24
CAS:	10287-53-3

Physical Properties

Property code	Value	Unit	Source
gf	21.38	kJ/mol	Joback Method
hf	-222.58	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	54.22	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.929		Crippen Method
mvol	159.510	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1711.00		NIST Webbook
rinpol	1711.00		NIST Webbook
tb	571.47	K	Joback Method
tc	778.84	K	Joback Method
tf	357.30	K	Joback Method
vc	0.586	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.59	J/molxK	571.47	Joback Method
cpg	396.33	J/molxK	606.03	Joback Method
cpg	410.24	J/molxK	640.59	Joback Method
cpg	423.33	J/molxK	675.15	Joback Method
cpg	435.62	J/molxK	709.72	Joback Method
cpg	447.15	J/molxK	744.28	Joback Method
cpg	457.93	J/molxK	778.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10287533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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