Benzoic acid, 2-(dimethylamino)ethyl ester

Other names:	2-(Dimethylaminoethyl)benzoate
	Quantacure DMB
Inchi:	InChI=1S/C11H15NO2/c1-12(2)8-9-14-11(13)10-6-4-3-5-7-10/h3-7H,8-9H2,1-2H3
InchiKey:	KJSGODDTWRXQRH-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CN(C)CCOC(=O)c1ccccc1
Mol. weight [g/mol]:	193.24
CAS:	2208-05-1

Physical Properties

Property code	Value	Unit	Source
gf	31.01	kJ/mol	Joback Method
hf	-211.11	kJ/mol	Joback Method
hfus	24.10	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.405		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	566.49	K	Joback Method
tc	772.84	K	Joback Method
tf	344.78	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.81	J/mol×K	566.49	Joback Method
cpg	396.83	J/mol×K	600.88	Joback Method
cpg	410.97	J/mol×K	635.27	Joback Method
cpg	424.25	J/mol×K	669.67	Joback Method
cpg	436.70	J/mol×K	704.06	Joback Method
cpg	448.35	J/mol×K	738.45	Joback Method
cpg	459.23	J/mol×K	772.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2208051&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume