Benzylpiperazine-M (desethylene-), 2AC

Inchi: InChI=1S/C13H18N2O2/c1-11(16)14-8-9-15(12(2)17)10-13-6-4-3-5-7-13/h3-7H,8-10H2,1
InchiKey: HRQWXMJJAOLWEO-UHFFFAOYSA-N
Formula: C13H18N2O2
SMILES: CC(=O)NCCN(Cc1ccccc1)C(C)=O
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	113.32	kJ/mol	Joback Method
hf	-179.28	kJ/mol	Joback Method
hfus	34.78	kJ/mol	Joback Method
hvap	68.78	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.171		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	2110.00		NIST Webbook
tb	693.87	K	Joback Method
tc	902.95	K	Joback Method
tf	447.68	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.58	J/mol×K	693.87	Joback Method
cpg	541.98	J/mol×K	728.72	Joback Method
cpg	555.40	J/mol×K	763.56	Joback Method
cpg	567.89	J/mol×K	798.41	Joback Method
cpg	579.49	J/mol×K	833.25	Joback Method
cpg	590.27	J/mol×K	868.10	Joback Method
cpg	600.27	J/mol×K	902.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R284289&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