2-Dimethylamino-8(ar)-methoxy-tetrahydro-1-acen

Inchi: InChI=1S/C16H21NO2/c1-17(2)9-12-11-6-4-5-10-7-8-13(19-3)15(14(10)11)16(12)18/h7-8
InchiKey: QXXUCXAVKQQQEZ-UHFFFAOYSA-N
Formula: C16H21NO2
SMILES: COc1ccc2c3c1C(=O)C(CN(C)C)C3CCC2
Mol. weight [g/mol]: 259.34
CAS: 116296-20-9

Physical Properties

Property code	Value	Unit	Source
gf	172.05	kJ/mol	Joback Method
hf	-228.24	kJ/mol	Joback Method
hfus	30.06	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.489		Crippen Method
mcvol	208.240	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
tb	723.26	K	Joback Method
tc	947.48	K	Joback Method
tf	492.86	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.97	J/mol×K	723.26	Joback Method
cpg	640.28	J/mol×K	760.63	Joback Method
cpg	657.42	J/mol×K	798.00	Joback Method
cpg	673.43	J/mol×K	835.37	Joback Method
cpg	688.40	J/mol×K	872.74	Joback Method
cpg	702.37	J/mol×K	910.11	Joback Method
cpg	715.40	J/mol×K	947.48	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=C116296209&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume