Beta-diethylamino ethyl ester of dicyclohexylamino acetic acid

Inchi: InChI=1S/C20H38N2O2/c1-3-21(4-2)15-16-24-20(23)17-22(18-11-7-5-8-12-18)19-13-9-6

InchiKey: JMAZNPAZWQLLKM-UHFFFAOYSA-N

Formula: C20H38N2O2

SMILES: CCN(CC)CCOC(=O)CN(C1CCCCC1)C1CCCCC1

Mol. weight [g/mol]: 338.53

CAS: 78546-03-9

Physical Properties

Property code	Value	Unit	Source
gf	154.06	kJ/mol	Joback Method
hf	-457.23	kJ/mol	Joback Method
hfus	40.05	kJ/mol	Joback Method
hvap	74.21	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.839		Crippen Method
mcvol	298.340	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
tb	797.27	K	Joback Method
tc	1002.53	K	Joback Method
tf	467.02	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.49	J/mol×K	797.27	Joback Method
cpg	1015.18	J/mol×K	831.48	Joback Method
cpg	1036.28	J/mol×K	865.69	Joback Method
cpg	1055.84	J/mol×K	899.90	Joback Method
cpg	1073.94	J/mol×K	934.11	Joback Method
cpg	1090.63	J/mol×K	968.32	Joback Method
cpg	1105.97	J/mol×K	1002.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78546039&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

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