N-(beta-dimethylaminoethyl) 3-bromo-2,2-diphenyl propionamide

Inchi: InChI=1S/C19H23BrN2O/c1-22(2)14-13-21-18(23)19(15-20,16-9-5-3-6-10-16)17-11-7-4-
InchiKey: JDLONZJRCXGEES-UHFFFAOYSA-N
Formula: C19H23BrN2O
SMILES: CN(C)CCNC(=O)C(CBr)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 375.30
CAS: 116402-45-0

Physical Properties

Property code	Value	Unit	Source
gf	422.33	kJ/mol	Joback Method
hf	63.57	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.045		Crippen Method
mcvol	270.080	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
tb	866.89	K	Joback Method
tc	1106.48	K	Joback Method
tf	554.01	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.60	J/mol×K	866.89	Joback Method
cpg	806.40	J/mol×K	906.82	Joback Method
cpg	820.12	J/mol×K	946.75	Joback Method
cpg	832.90	J/mol×K	986.69	Joback Method
cpg	844.91	J/mol×K	1026.62	Joback Method
cpg	856.31	J/mol×K	1066.55	Joback Method
cpg	867.25	J/mol×K	1106.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402450&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