«beta»-Alanine, N-(2-bromobenzoyl)-, decyl ester

Inchi: InChI=1S/C20H30BrNO3/c1-2-3-4-5-6-7-8-11-16-25-19(23)14-15-22-20(24)17-12-9-10-1

InchiKey: XCCAPTHWPPTKGA-UHFFFAOYSA-N

Formula: C20H30BrNO3

SMILES: CCCCCCCCCCOC(=O)CCNC(=O)c1ccccc1Br

Mol. weight [g/mol]: 412.36

Physical Properties

Property code	Value	Unit	Source
gf	-38.83	kJ/mol	Joback Method
hf	-508.65	kJ/mol	Joback Method
hfus	55.98	kJ/mol	Joback Method
hvap	91.82	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.253		Crippen Method
mcvol	305.390	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	3052.00		NIST Webbook
rinpol	3052.00		NIST Webbook
tb	935.15	K	Joback Method
tc	1150.57	K	Joback Method
tf	588.65	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.11	J/mol×K	935.15	Joback Method
cpg	961.37	J/mol×K	971.05	Joback Method
cpg	974.55	J/mol×K	1006.96	Joback Method
cpg	986.70	J/mol×K	1042.86	Joback Method
cpg	997.88	J/mol×K	1078.76	Joback Method
cpg	1008.14	J/mol×K	1114.66	Joback Method
cpg	1017.55	J/mol×K	1150.57	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=U321734&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume