D-Alanine, N-(4-butylbenzoyl)-, isohexyl ester

Inchi: InChI=1S/C20H31NO3/c1-5-6-9-17-10-12-18(13-11-17)19(22)21-16(4)20(23)24-14-7-8-1
InchiKey: FATRVLFVVZDRLX-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CCCCc1ccc(C(=O)NC(C)C(=O)OCCCC(C)C)cc1
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
gf	-58.03	kJ/mol	Joback Method
hf	-545.54	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	84.61	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.127		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
rinpol	2575.00		NIST Webbook
tb	868.11	K	Joback Method
tc	1074.99	K	Joback Method
tf	498.85	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.00	J/mol×K	868.11	Joback Method
cpg	925.01	J/mol×K	902.59	Joback Method
cpg	939.86	J/mol×K	937.07	Joback Method
cpg	953.58	J/mol×K	971.55	Joback Method
cpg	966.22	J/mol×K	1006.03	Joback Method
cpg	977.81	J/mol×K	1040.51	Joback Method
cpg	988.39	J/mol×K	1074.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354100&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume