«beta»-Alanine, N-(2-methylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C18H27NO3/c1-3-4-5-6-9-14-22-17(20)12-13-19-18(21)16-11-8-7-10-15(16)2/l
InchiKey: YSDYTFNZBZPWMW-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CCCCCCCOC(=O)CCNC(=O)c1ccccc1C
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-69.99	kJ/mol	Joback Method
hf	-493.70	kJ/mol	Joback Method
hfus	45.51	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.629		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2459.00		NIST Webbook
tb	823.23	K	Joback Method
tc	1025.77	K	Joback Method
tf	506.31	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.71	J/mol×K	823.23	Joback Method
cpg	806.04	J/mol×K	856.99	Joback Method
cpg	820.33	J/mol×K	890.74	Joback Method
cpg	833.61	J/mol×K	924.50	Joback Method
cpg	845.91	J/mol×K	958.26	Joback Method
cpg	857.27	J/mol×K	992.01	Joback Method
cpg	867.73	J/mol×K	1025.77	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321618&Units=SI

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

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