Benalaxyl

Other names: DL-Alanine, N-(2,6-dimethylphenyl)-N-(phenylacetyl)-, methyl ester
Alanine, N-(2,6-dimethylphenyl)-N-(phenylacetyl)-, methyl ester, dl-
Galben
M 9834
methyl N-(2,6-dimethylphenyl)-N-(phenylacetyl)-DL-alaninate
Inchi: InChI=1S/C20H23NO3/c1-14-9-8-10-15(2)19(14)21(16(3)20(23)24-4)18(22)13-17-11-6-5
InchiKey: CJPQIRJHIZUAQP-UHFFFAOYSA-N
Formula: C20H23NO3
SMILES: COC(=O)C(C)N(C(=O)Cc1ccccc1)c1c(C)cccc1C
Mol. weight [g/mol]: 325.40
CAS: 71626-11-4

Physical Properties

Property code	Value	Unit	Source
gf	68.58	kJ/mol	Joback Method
hf	-301.14	kJ/mol	Joback Method
hfus	38.74	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.441		Crippen Method
mcvol	264.130	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2334.00		NIST Webbook
rinpol	2334.00		NIST Webbook
tb	862.48	K	Joback Method
tc	1089.34	K	Joback Method
tf	532.60	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.95	J/mol×K	862.48	Joback Method
cpg	809.81	J/mol×K	900.29	Joback Method

cpg	823.41	J/mol×K	938.10	Joback Method
cpg	835.82	J/mol×K	975.91	Joback Method
cpg	847.08	J/mol×K	1013.72	Joback Method
cpg	857.27	J/mol×K	1051.53	Joback Method
cpg	866.45	J/mol×K	1089.34	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=C71626114&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