«beta»-Alanine, N-(4-ethylbenzoyl)-, octyl ester

Inchi: InChI=1S/C20H31NO3/c1-3-5-6-7-8-9-16-24-19(22)14-15-21-20(23)18-12-10-17(4-2)11-
InchiKey: JWPCAGBPCUAEKQ-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CCCCCCCCOC(=O)CCNC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
gf	-53.15	kJ/mol	Joback Method
hf	-534.98	kJ/mol	Joback Method
hfus	50.69	kJ/mol	Joback Method
hvap	85.39	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.273		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	2729.00		NIST Webbook
rinpol	2729.00		NIST Webbook
tb	868.99	K	Joback Method
tc	1072.63	K	Joback Method
tf	528.85	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.99	J/mol×K	868.99	Joback Method
cpg	923.79	J/mol×K	902.93	Joback Method
cpg	938.49	J/mol×K	936.87	Joback Method
cpg	952.12	J/mol×K	970.81	Joback Method
cpg	964.71	J/mol×K	1004.75	Joback Method
cpg	976.31	J/mol×K	1038.69	Joback Method
cpg	986.96	J/mol×K	1072.63	Joback Method

Sources

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=U321656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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