1-(4-Aminophenyl)-2-(4-butyrylphenyl)ethane

Inchi: InChI=1S/C18H21NO/c1-2-3-18(20)16-10-6-14(7-11-16)4-5-15-8-12-17(19)13-9-15/h6-1
InchiKey: QNTHPWZRRASATN-UHFFFAOYSA-N
Formula: C18H21NO
SMILES: CCCC(=O)c1ccc(CCc2ccc(N)cc2)cc1
Mol. weight [g/mol]: 267.37
CAS: 17438-50-5

Physical Properties

Property code	Value	Unit	Source
gf	243.77	kJ/mol	Joback Method
hf	-43.52	kJ/mol	Joback Method
hfus	36.48	kJ/mol	Joback Method
hvap	78.92	kJ/mol	Joback Method
ie	8.10 ± 0.20	eV	NIST Webbook
log10ws	-5.02		Crippen Method
logp	4.037		Crippen Method
mcvol	228.510	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
tb	800.96	K	Joback Method
tc	1035.28	K	Joback Method
tf	503.69	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.46	J/mol×K	800.96	Joback Method
cpg	677.95	J/mol×K	840.01	Joback Method
cpg	692.26	J/mol×K	879.07	Joback Method
cpg	705.45	J/mol×K	918.12	Joback Method
cpg	717.60	J/mol×K	957.17	Joback Method
cpg	728.79	J/mol×K	996.22	Joback Method
cpg	739.09	J/mol×K	1035.28	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=C17438505&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume