1-(4-Butyrylphenyl)-2-(4-nitrophenyl)ethane

Inchi: InChI=1S/C18H19NO3/c1-2-3-18(20)16-10-6-14(7-11-16)4-5-15-8-12-17(13-9-15)19(21)
InchiKey: HQXSMDGREYUOEZ-UHFFFAOYSA-N
Formula: C18H19NO3
SMILES: CCCC(=O)c1ccc(CCc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 297.35
CAS: 17302-70-4

Physical Properties

Property code	Value	Unit	Source
gf	212.87	kJ/mol	Joback Method
hf	-88.07	kJ/mol	Joback Method
hfus	42.64	kJ/mol	Joback Method
hvap	84.88	kJ/mol	Joback Method
ie	9.10 ± 0.20	eV	NIST Webbook
log10ws	-6.04		Crippen Method
logp	4.363		Crippen Method
mcvol	235.950	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
tb	880.27	K	Joback Method
tc	1126.60	K	Joback Method
tf	564.04	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.54	J/mol×K	880.27	Joback Method
cpg	717.17	J/mol×K	921.33	Joback Method
cpg	729.63	J/mol×K	962.38	Joback Method
cpg	741.00	J/mol×K	1003.44	Joback Method
cpg	751.37	J/mol×K	1044.49	Joback Method
cpg	760.83	J/mol×K	1085.55	Joback Method
cpg	769.46	J/mol×K	1126.60	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=C17302704&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