Naproanilide

Inchi: InChI=1S/C19H17NO2/c1-14(19(21)20-17-9-3-2-4-10-17)22-18-12-11-15-7-5-6-8-16(15)
InchiKey: LVKTWOXHRYGDMM-UHFFFAOYSA-N
Formula: C19H17NO2
SMILES: CC(Oc1ccc2ccccc2c1)C(=O)Nc1ccccc1
Mol. weight [g/mol]: 291.34
CAS: 51888-81-4

Physical Properties

Property code	Value	Unit	Source
gf	283.97	kJ/mol	Joback Method
hf	20.56	kJ/mol	Joback Method
hfus	34.04	kJ/mol	Joback Method
hvap	79.95	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.246		Crippen Method
mcvol	229.010	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	837.46	K	Joback Method
tc	1085.05	K	Joback Method
tf	511.77	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.09	J/mol×K	837.46	Joback Method
cpg	678.35	J/mol×K	878.72	Joback Method
cpg	691.39	J/mol×K	919.99	Joback Method
cpg	703.32	J/mol×K	961.25	Joback Method
cpg	714.27	J/mol×K	1002.52	Joback Method
cpg	724.34	J/mol×K	1043.78	Joback Method
cpg	733.65	J/mol×K	1085.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51888814&Units=SI
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

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