

Tolfenamic acid

Other names:

Benzoic acid, 2-[(3-chloro-2-methylphenyl)amino]-
Anthranilic acid, N-(3-chloro-o-tolyl)-
N-(3-Chloro-2-methylphenyl)anthranilic acid
N-(3-Chloro-o-tolyl)-anthranilic acid
GEA 6414
N-(2-Methyl-3-chlorophenyl)anthranilic acid
Clotam
Tolfedine
Tolfine
2-[(3-Chloro-2-methylphenyl)amino]benzoic acid (tolfenamic acid)

Inchi: InChI=1S/C14H12ClNO2/c1-9-11(15)6-4-8-12(9)16-13-7-3-2-5-10(13)14(17)18/h2-8,16H**InchiKey:** YEZNLOUZAIOMLT-UHFFFAOYSA-N**Formula:** C14H12ClNO2**SMILES:** Cc1c(Cl)cccc1Nc1ccccc1C(=O)O**Mol. weight [g/mol]:** 261.70**CAS:** 13710-19-5

Physical Properties

Property code	Value	Unit	Source
gf	74.65	kJ/mol	Joback Method
hf	-120.72	kJ/mol	Joback Method
hfus	33.91	kJ/mol	Joback Method
hsub	128.40 ± 0.80	kJ/mol	NIST Webbook
hvap	87.54	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.090		Crippen Method
mcvol	190.260	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	821.67	K	Joback Method
tc	1051.15	K	Joback Method
tf	531.27	K	Joback Method
vc	0.713	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.60	J/mol×K	1012.90	Joback Method
cpg	507.69	J/mol×K	821.67	Joback Method
cpg	517.86	J/mol×K	859.92	Joback Method
cpg	527.18	J/mol×K	898.16	Joback Method
cpg	535.71	J/mol×K	936.41	Joback Method
cpg	543.50	J/mol×K	974.66	Joback Method
cpg	557.07	J/mol×K	1051.15	Joback Method
hfust	38.60	kJ/mol	484.30	NIST Webbook
hfust	41.20	kJ/mol	485.30	NIST Webbook
hsubt	125.70 ± 0.80	kJ/mol	359.50	NIST Webbook

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=C13710195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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