Benzoic acid, 2-[[(3-methylphenyl)amino]carbonyl]-

Other names: Phthalanilic acid, 3'-methyl-
Duraset
Duraset 20W
N-m-Tolylphthalamic acid
N-m-Tolylphthalaminic acid
N-m-t
N-Metatolyl phthalamic acid
Phthalamate
Tomaset
3'-Methylphthalanilic acid
Kyselina N-m-tolylftalamova
2-(((3-Methylphenyl)amino)carbonyl)benzoic acid
NSC 522078

Inchi: InChI=1S/C15H13NO3/c1-10-5-4-6-11(9-10)16-14(17)12-7-2-3-8-13(12)15(18)19/h2-9H,

InchiKey: AZPJXONNBLOZFE-UHFFFAOYSA-N

Formula: C15H13NO3

SMILES: Cc1cccc(NC(=O)c2ccccc2C(=O)O)c1

Mol. weight [g/mol]: 255.27

CAS: 85-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-24.29	kJ/mol	Joback Method
hf	-226.73	kJ/mol	Joback Method
hfus	34.29	kJ/mol	Joback Method
hvap	91.47	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.946		Crippen Method
mcvol	193.680	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	856.01	K	Joback Method
tc	1084.59	K	Joback Method
tf	550.03	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.01	J/mol×K	856.01	Joback Method
cpg	560.10	J/mol×K	894.11	Joback Method
cpg	569.30	J/mol×K	932.20	Joback Method
cpg	577.67	J/mol×K	970.30	Joback Method
cpg	585.27	J/mol×K	1008.39	Joback Method
cpg	592.16	J/mol×K	1046.49	Joback Method
cpg	598.40	J/mol×K	1084.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85723&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume