Pyracarbolid

Other names: 2-Methyl-5,6-dihydro-4,4-pyran-3-carbonsaeureanilid
2-Methyl-5,6-dihydro-4-H-pyrane-3-carboxylic acid anilide
2H-Pyran-5-carboxamide, 3,4-dihydro-6-methyl-N-phenyl-
2H-Pyran-5-carboxanilide, 3,4-dihydro-6-methyl-
3,4-Dihydro-6-methyl-2H-pyran-5-carboxanilide
3,4-Dihydro-6-methyl-N-phenyl-2H-pyran-5-carboxamide
4H-Pyran, 5,6-dihydro-2-methyl-3-(phenylcarbamoyl)-
5-6-Dihydro-2-methyl-3-(phenylcarbamoyl)-4H-pyrane
HOE 13764
HOE 13764 OF
HOE 2989
HOE 6052
HOE 6053
Pyracarbolide
Sicarol

Inchi: InChI=1S/C13H15NO2/c1-10-12(8-5-9-16-10)13(15)14-11-6-3-2-4-7-11/h2-4,6-7H,5,8-9H

InchiKey: YPCALTGLHFLNGA-UHFFFAOYSA-N

Formula: C13H15NO2

SMILES: CC1=C(C(=O)Nc2ccccc2)CCCO1

Mol. weight [g/mol]: 217.26

CAS: 24691-76-7

Physical Properties

Property code	Value	Unit	Source
gf	88.20	kJ/mol	Joback Method
hf	-156.73	kJ/mol	Joback Method
hfus	29.35	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Joback Method
log10ws	-2.56		Estimated Solubility Method
log10ws	-2.56		Aqueous Solubility Prediction Method
logp	2.710		Crippen Method
mcvol	172.530	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	687.85	K	Joback Method
tc	929.57	K	Joback Method

tf	381.40 ± 0.20	K	NIST Webbook
tf	383.65	K	Aqueous Solubility Prediction Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.30	J/mol×K	849.00	Joback Method
cpg	532.41	J/mol×K	889.28	Joback Method
cpg	465.60	J/mol×K	687.85	Joback Method
cpg	481.34	J/mol×K	728.14	Joback Method
cpg	495.82	J/mol×K	768.42	Joback Method
cpg	509.12	J/mol×K	808.71	Joback Method
cpg	542.51	J/mol×K	929.57	Joback Method
hfust	19.21	kJ/mol	381.10	NIST Webbook
hfust	19.21	kJ/mol	381.10	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24691767&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
hfust: Enthalpy of fusion 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