4-Propylbiphenyl-4'-carboxylic acid

Other names: 4-n-Propylbiphenyl-4'-carboxylic acid
4-(4-n-Propylphenyl)benzoic acid
4-(p-n-Propylphenyl)benzoic acid
Inchi: InChI=1S/C16H16O2/c1-2-3-12-4-6-13(7-5-12)14-8-10-15(11-9-14)16(17)18/h4-11H,2-3H
InchiKey: HCPBURTZSXRGBN-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: CCCc1ccc(-c2ccc(C(=O)O)cc2)cc1
Mol. weight [g/mol]: 240.30
CAS: 88038-94-2

Physical Properties

Property code	Value	Unit	Source
gf	23.66	kJ/mol	Joback Method
hf	-188.26	kJ/mol	Joback Method
hfus	30.19	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.004		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	774.85	K	Joback Method
tc	995.30	K	Joback Method
tf	458.71	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.68	J/mol×K	774.85	Joback Method
cpg	557.44	J/mol×K	811.59	Joback Method
cpg	569.26	J/mol×K	848.33	Joback Method
cpg	580.20	J/mol×K	885.08	Joback Method
cpg	590.31	J/mol×K	921.82	Joback Method
cpg	599.66	J/mol×K	958.56	Joback Method

cpg	608.29	J/mol×K	995.30	Joback Method
dvisc	0.0008732	Pa×s	458.71	Joback Method
dvisc	0.0003764	Pa×s	511.40	Joback Method
dvisc	0.0001898	Pa×s	564.09	Joback Method
dvisc	0.0001076	Pa×s	616.78	Joback Method
dvisc	0.0000667	Pa×s	669.47	Joback Method
dvisc	0.0000444	Pa×s	722.16	Joback Method
dvisc	0.0000312	Pa×s	774.85	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88038942&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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