

Butyric acid, ester with p-hydroxybenzonitrile

Other names:	4-Cyanophenyl butyrate Butyric acid, 4-cyanophenyl ester
Inchi:	InChI=1S/C11H11NO2/c1-2-3-11(13)14-10-6-4-9(8-12)5-7-10/h4-7H,2-3H2,1H3
InchiKey:	UQWSXHNINZRCTC-UHFFFAOYSA-N
Formula:	C11H11NO2
SMILES:	CCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]:	189.21
CAS:	29052-10-6

Physical Properties

Property code	Value	Unit	Source
gf	43.78	kJ/mol	Joback Method
hf	-125.23	kJ/mol	Joback Method
hfus	22.19	kJ/mol	Joback Method
hvap	62.65	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.264		Crippen Method
mcvol	150.910	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	661.11	K	Joback Method
tc	885.39	K	Joback Method
tf	389.82	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.89	J/mol×K	661.11	Joback Method
cpg	382.46	J/mol×K	698.49	Joback Method
cpg	393.27	J/mol×K	735.87	Joback Method
cpg	403.33	J/mol×K	773.25	Joback Method
cpg	412.66	J/mol×K	810.63	Joback Method

cpg	421.28	J/mol×K	848.01	Joback Method
cpg	429.19	J/mol×K	885.39	Joback Method

Sources

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=C29052106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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