

Valeric acid, 4-cyanophenyl ester

Inchi:	InChI=1S/C12H13NO2/c1-2-3-4-12(14)15-11-7-5-10(9-13)6-8-11/h5-8H,2-4H2,1H3
InchiKey:	MMIDKFMIMXKQFT-UHFFFAOYSA-N
Formula:	C12H13NO2
SMILES:	CCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]:	203.24

Physical Properties

Property code	Value	Unit	Source
gf	52.20	kJ/mol	Joback Method
hf	-145.87	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.654		Crippen Method
mcvol	165.000	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	683.99	K	Joback Method
tc	904.34	K	Joback Method
tf	401.09	K	Joback Method
vc	0.649	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.49	J/mol×K	683.99	Joback Method
cpg	432.73	J/mol×K	720.72	Joback Method
cpg	444.17	J/mol×K	757.44	Joback Method
cpg	454.83	J/mol×K	794.17	Joback Method
cpg	464.71	J/mol×K	830.89	Joback Method
cpg	473.85	J/mol×K	867.62	Joback Method
cpg	482.26	J/mol×K	904.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U307987&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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