3-Methylbut-2-enoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C12H11NO2/c1-9(2)7-12(14)15-11-5-3-10(8-13)4-6-11/h3-7H,1-2H3
InchiKey: KQIOMMKFZCDOIT-UHFFFAOYSA-N
Formula: C12H11NO2
SMILES: CC(C)=CC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 201.22

Physical Properties

Property code	Value	Unit	Source
gf	123.87	kJ/mol	Joback Method
hf	-38.44	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	64.92	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.430		Crippen Method
mcvol	160.700	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1653.00		NIST Webbook
rinpol	1653.00		NIST Webbook
tb	688.03	K	Joback Method
tc	920.86	K	Joback Method
tf	382.05	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.98	J/mol×K	688.03	Joback Method
cpg	408.71	J/mol×K	726.83	Joback Method
cpg	419.61	J/mol×K	765.64	Joback Method
cpg	429.72	J/mol×K	804.44	Joback Method
cpg	439.07	J/mol×K	843.25	Joback Method
cpg	447.71	J/mol×K	882.05	Joback Method
cpg	455.68	J/mol×K	920.86	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=U307596&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