4-Cyanobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C18H19NO2/c1-13(2)5-10-17(11-14(3)4)21-18(20)16-8-6-15(12-19)7-9-16/h6-9
InchiKey: NUJGCPSYGPBEBN-UHFFFAOYSA-N
Formula: C18H19NO2
SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
gf	379.93	kJ/mol	Joback Method
hf	107.67	kJ/mol	Joback Method
hfus	33.81	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.709		Crippen Method
mcvol	236.640	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	2005.00		NIST Webbook
tb	825.95	K	Joback Method
tc	1060.94	K	Joback Method
tf	529.09	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.00	J/mol×K	825.95	Joback Method
cpg	681.11	J/mol×K	865.11	Joback Method
cpg	694.12	J/mol×K	904.28	Joback Method
cpg	706.08	J/mol×K	943.44	Joback Method
cpg	717.02	J/mol×K	982.61	Joback Method
cpg	727.01	J/mol×K	1021.77	Joback Method
cpg	736.08	J/mol×K	1060.94	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=U299227&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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