4-Cyanobenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H19NO2/c1-4-5-6-16(11-13(2)3)20-17(19)15-9-7-14(12-18)8-10-15/h7-10,1

InchiKey: MOIOXTMHXLNGKS-UHFFFAOYSA-N

Formula: C17H19NO2

SMILES: CCC#CC(CC(C)C)OC(=O)c1ccc(C#N)cc1

Mol. weight [g/mol]: 269.34

Physical Properties

Property code	Value	Unit	Source
gf	292.22	kJ/mol	Joback Method
hf	12.67	kJ/mol	Joback Method
hfus	33.81	kJ/mol	Joback Method
hvap	77.38	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	3.543		Crippen Method
mcvol	226.850	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tb	806.51	K	Joback Method
tc	1038.13	K	Joback Method
tf	533.54	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.22	J/mol×K	806.51	Joback Method
cpg	652.42	J/mol×K	845.11	Joback Method
cpg	665.53	J/mol×K	883.72	Joback Method
cpg	677.58	J/mol×K	922.32	Joback Method
cpg	688.61	J/mol×K	960.92	Joback Method
cpg	698.65	J/mol×K	999.53	Joback Method
cpg	707.73	J/mol×K	1038.13	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=U299226&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