

4-Cyanobenzoic acid, tridec-2-ynyl ester

Inchi:	InChI=1S/C21H27NO2/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-21(23)20-15-13-19(18-22)14-
InchiKey:	OEEANJGYVSZIIIE-UHFFFAOYSA-N
Formula:	C21H27NO2
SMILES:	CCCCCCCCC#CCOC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]:	325.44

Physical Properties

Property code	Value	Unit	Source
gf	330.78	kJ/mol	Joback Method
hf	-59.33	kJ/mol	Joback Method
hfus	51.21	kJ/mol	Joback Method
hvap	87.06	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	5.249		Crippen Method
mvol	283.210	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	898.91	K	Joback Method
tc	1116.94	K	Joback Method
tf	608.62	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.71	J/mol×K	898.91	Joback Method
cpg	880.46	J/mol×K	935.25	Joback Method
cpg	894.11	J/mol×K	971.59	Joback Method
cpg	906.71	J/mol×K	1007.93	Joback Method
cpg	918.30	J/mol×K	1044.27	Joback Method
cpg	928.93	J/mol×K	1080.61	Joback Method
cpg	938.64	J/mol×K	1116.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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=U299230&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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