

4-Chlorobenzoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi:	InChI=1S/C18H21ClO2/c1-5-6-14(4)17(12-7-13(2)3)21-18(20)15-8-10-16(19)11-9-15/h8-
InchiKey:	VSKMPLKDSXMUOU-UHFFFAOYSA-N
Formula:	C18H21ClO2
SMILES:	<chem>C=C(C)C#CC(OC(=O)c1ccc(Cl)cc1)C(C)CCC</chem>
Mol. weight [g/mol]:	304.81

Physical Properties

Property code	Value	Unit	Source
gf	234.82	kJ/mol	Joback Method
hf	-72.95	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	72.93	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.881		Crippen Method
mcvol	247.500	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
tb	761.30	K	Joback Method
tc	988.45	K	Joback Method
tf	494.02	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.84	J/molxK	761.30	Joback Method
cpg	685.10	J/molxK	799.16	Joback Method
cpg	700.22	J/molxK	837.02	Joback Method
cpg	714.24	J/molxK	874.88	Joback Method
cpg	727.21	J/molxK	912.74	Joback Method
cpg	739.18	J/molxK	950.59	Joback Method
cpg	750.19	J/molxK	988.45	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=U299369&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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