

exo-2-(1,1-Dimethylpent-2-yn-4-enyloxycarbonyl)k

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H18O2/c1-4-5-8-15(2,3)17-14(16)13-10-11-6-7-12(13)9-11/h4,6-7,11-13H,

CUXQPFYTGKBHMG-LKOMHFJYSA-N

C15H18O2

C=CC#CC(C)(C)OC(=O)C1CC2C=CC1C2

230.30

Physical Properties

Property code	Value	Unit	Source
gf	266.63	kJ/mol	Joback Method
hf	-31.87	kJ/mol	Joback Method
hfus	28.28	kJ/mol	Joback Method
hvap	58.31	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.710		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
tb	633.58	K	Joback Method
tc	865.81	K	Joback Method
tf	466.61	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.36	J/mol×K	633.58	Joback Method
cpg	534.07	J/mol×K	672.29	Joback Method
cpg	551.43	J/mol×K	710.99	Joback Method
cpg	567.55	J/mol×K	749.70	Joback Method
cpg	582.52	J/mol×K	788.40	Joback Method
cpg	596.48	J/mol×K	827.11	Joback Method
cpg	609.51	J/mol×K	865.81	Joback Method

Sources

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=R507463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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