

Falcarinone

Other names:	Panaxynone
Inchi:	InChI=1S/C17H22O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17(18)4-2/h4,10-11H,2-3,5-9,17H
InchiKey:	UQEBOJRXTNLPKZ-KHPPLWFESA-N
Formula:	C17H22O
SMILES:	<chem>C=CC(=O)C#CC#CCC=CCCCCCCC</chem>
Mol. weight [g/mol]:	242.36
CAS:	4117-11-7

Physical Properties

Property code	Value	Unit	Source
gf	537.00	kJ/mol	Joback Method
hf	280.46	kJ/mol	Joback Method
hfus	46.55	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.055		Crippen Method
mcvol	226.160	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2018.40		NIST Webbook
rinpol	2018.40		NIST Webbook
tb	661.07	K	Joback Method
tc	870.79	K	Joback Method
tf	536.64	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.82	J/molxK	661.07	Joback Method
cpg	590.67	J/molxK	696.02	Joback Method
cpg	606.60	J/molxK	730.98	Joback Method
cpg	621.67	J/molxK	765.93	Joback Method
cpg	635.91	J/molxK	800.89	Joback Method
cpg	649.39	J/molxK	835.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4117117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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