

6-Acetoxy-11-nor-drim-7-en-9-one

Inchi:	InChI=1S/C16H24O3/c1-10-9-12(19-11(2)17)13-15(3,4)7-6-8-16(13,5)14(10)18/h9,12-13
InchiKey:	GRFRYZCZEBLHGL-UHFFFAOYSA-N
Formula:	C16H24O3
SMILES:	CC(=O)OC1C=C(C)C(=O)C2(C)CCCC(C)(C)C12
Mol. weight [g/mol]:	264.36
CAS:	220766-77-8

Physical Properties

Property code	Value	Unit	Source
gf	-205.64	kJ/mol	Joback Method
hf	-599.00	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	63.16	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.280		Crippen Method
mcvol	219.290	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1815.10		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1815.10		NIST Webbook
rinpol	1778.00		NIST Webbook
ripol	2457.00		NIST Webbook
ripol	2457.00		NIST Webbook
tb	735.43	K	Joback Method
tc	970.85	K	Joback Method
tf	484.86	K	Joback Method
vc	0.825	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.78	J/mol×K	735.43	Joback Method
cpg	693.37	J/mol×K	774.67	Joback Method
cpg	714.32	J/mol×K	813.90	Joback Method

cpg	734.85	J/mol×K	853.14	Joback Method
cpg	755.18	J/mol×K	892.37	Joback Method
cpg	775.52	J/mol×K	931.61	Joback Method
cpg	796.09	J/mol×K	970.85	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=C220766778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/89-739-4/6-Acetoxy-11-nor-drim-7-en-9-one.pdf>

Generated by Cheméo on 2024-04-19 21:40:42.618239303 +0000 UTC m=+15852091.538816624.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.