

(-)-(7R,10S)-eudesm-4-en-6-one

Inchi:	InChI=1S/C15H24O/c1-10(2)12-7-9-15(4)8-5-6-11(3)13(15)14(12)16/h10,12H,5-9H2,1-4H
InchiKey:	LRSNSCWFOBGPBP-WFASDCNBSA-N
Formula:	C15H24O
SMILES:	CC1=C2C(=O)C(C(C)C)CCC2(C)CCC1
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	28.70	kJ/mol	Joback Method
hf	-324.87	kJ/mol	Joback Method
hfus	12.61	kJ/mol	Joback Method
hvap	53.82	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.128		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinsol	1605.00		NIST Webbook
tb	649.90	K	Joback Method
tc	884.41	K	Joback Method
tf	383.53	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.93	J/molxK	649.90	Joback Method
cpg	584.17	J/molxK	688.99	Joback Method
cpg	605.19	J/molxK	728.07	Joback Method
cpg	625.15	J/molxK	767.16	Joback Method
cpg	644.17	J/molxK	806.24	Joback Method
cpg	662.39	J/molxK	845.33	Joback Method
cpg	679.96	J/molxK	884.41	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=R422887&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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