

Musk galaxolide

Other names:	Galaxolide
Inchi:	InChI=1S/C18H26O/c1-11-9-19-10-13-7-15-16(8-14(11)13)18(5,6)12(2)17(15,3)4/h7-8,1
InchiKey:	ONKNPOPIGWHAQC-UHFFFAOYSA-N
Formula:	C18H26O
SMILES:	CC1COCc2cc3c(cc21)C(C)(C)C(C)C3(C)C
Mol. weight [g/mol]:	258.40

Physical Properties

Property code	Value	Unit	Source
gf	181.08	kJ/mol	Joback Method
hf	-215.49	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	61.51	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.525		Crippen Method
mcvol	224.870	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1818.50		NIST Webbook
rinpol	1846.90		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1818.50		NIST Webbook
rinpol	1819.20		NIST Webbook
rinpol	1846.90		NIST Webbook
tb	688.70	K	Joback Method
tc	920.33	K	Joback Method
tf	454.85	K	Joback Method
vc	0.857	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.21	J/molxK	688.70	Joback Method
cpg	681.77	J/molxK	727.30	Joback Method

cpg	702.55	J/mol×K	765.91	Joback Method
cpg	722.86	J/mol×K	804.51	Joback Method
cpg	742.99	J/mol×K	843.12	Joback Method
cpg	763.23	J/mol×K	881.72	Joback Method
cpg	783.89	J/mol×K	920.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R176564&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
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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