

Tonalid

Other names:	Ethanone, 1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthalenyl)- Tonalide Musk tonalid 1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one
Inchi:	InChI=1S/C18H26O/c1-11-8-16-15(9-14(11)13(3)19)17(4,5)10-12(2)18(16,6)7/h8-9,12H,
InchiKey:	DNRJTBAOUJJKDY-UHFFFAOYSA-N
Formula:	C18H26O
SMILES:	<chem>CC(=O)c1cc2c(cc1C)C(C)(C)C(C)CC2(C)C</chem>
Mol. weight [g/mol]:	258.40
CAS:	21145-77-7

Physical Properties

Property code	Value	Unit	Source
gf	77.53	kJ/mol	Joback Method
hf	-268.87	kJ/mol	Joback Method
hfus	22.43	kJ/mol	Joback Method
hvap	63.83	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.793		Crippen Method
mcvol	231.430	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2373.00		NIST Webbook
tb	708.88	K	Joback Method
tc	934.66	K	Joback Method
tf	329.50 ± 0.50	K	NIST Webbook
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.77	J/mol×K	708.88	Joback Method
cpg	685.10	J/mol×K	746.51	Joback Method
cpg	704.85	J/mol×K	784.14	Joback Method
cpg	724.26	J/mol×K	821.77	Joback Method
cpg	743.56	J/mol×K	859.40	Joback Method
cpg	763.00	J/mol×K	897.03	Joback Method
cpg	782.81	J/mol×K	934.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.00	K	0.20	NIST Webbook
tbrp	392.00	K	0.03	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21145777&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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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