trans-Calamenen-10-ol

Inchi: InChI=1S/C15H22O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h5-6,9-10,12,16H,7-
InchiKey: MTOMOICLIZNIAM-DOMZBBRYSA-N
Formula: C15H22O
SMILES: Cc1ccc2c(c1)C(C(C)C)CCC2(C)O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	64.76	kJ/mol	Joback Method
hf	-235.31	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	67.50	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.736		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1669.00		NIST Webbook
tb	677.56	K	Joback Method
tc	887.88	K	Joback Method
tf	390.17	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.94	J/mol×K	677.56	Joback Method

cpg	563.77	J/mol×K	712.61	Joback Method
cpg	579.80	J/mol×K	747.67	Joback Method
cpg	595.17	J/mol×K	782.72	Joback Method
cpg	610.00	J/mol×K	817.77	Joback Method
cpg	624.42	J/mol×K	852.83	Joback Method
cpg	638.55	J/mol×K	887.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411199&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