Cadina-1(10),6,8-triene

Other names: 8-Isopropyl-2,5-dimethyltetralin
Calamene
Inchi: InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h6,8,10-11H,5,7,9H2,1-4
InchiKey: LVIDDMJSLAVTSZ-UHFFFAOYSA-N
Formula: C15H22
SMILES: Cc1ccc(C(C)C)c2c1CCC(C)C2
Mol. weight [g/mol]: 202.34
CAS: 1460-96-4

Physical Properties

Property code	Value	Unit	Source
gf	205.15	kJ/mol	Joback Method
hf	-89.45	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.243		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1519.00		NIST Webbook

rinpol	1527.00		NIST Webbook
rinpol	1519.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1876.00		NIST Webbook
tb	594.79	K	Joback Method
tc	814.30	K	Joback Method
tf	322.21	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.12	J/mol×K	594.79	Joback Method
cpg	571.28	J/mol×K	777.72	Joback Method
cpg	555.62	J/mol×K	741.13	Joback Method
cpg	538.92	J/mol×K	704.55	Joback Method
cpg	521.14	J/mol×K	667.96	Joback Method
cpg	502.23	J/mol×K	631.38	Joback Method
cpg	585.98	J/mol×K	814.30	Joback Method
dvisc	0.0002663	Pa×s	594.79	Joback Method
dvisc	0.0003208	Pa×s	549.36	Joback Method
dvisc	0.0003995	Pa×s	503.93	Joback Method
dvisc	0.0005197	Pa×s	458.50	Joback Method
dvisc	0.0007164	Pa×s	413.07	Joback Method
dvisc	0.0010690	Pa×s	367.64	Joback Method
dvisc	0.0017856	Pa×s	322.21	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1460964&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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