Lactarazulene

Inchi: InChI=1S/C15H16/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h5-9H,1H2,2-4H3
InchiKey: KFLXZUPIDNPCSD-UHFFFAOYSA-N
Formula: C15H16
SMILES: C=C(C)c1ccc(C)c2ccc(C)c-2c1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	344.88	kJ/mol	Joback Method
hf	155.90	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	54.30	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.441		Crippen Method
mcvol	174.690	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1796.00		NIST Webbook
ripol	2430.00		NIST Webbook
tb	599.76	K	Joback Method
tc	828.44	K	Joback Method
tf	339.77	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.47	J/mol×K	599.76	Joback Method
cpg	433.79	J/mol×K	637.87	Joback Method
cpg	449.04	J/mol×K	675.99	Joback Method
cpg	463.30	J/mol×K	714.10	Joback Method
cpg	476.64	J/mol×K	752.21	Joback Method
cpg	489.14	J/mol×K	790.33	Joback Method

cpg	500.86	J/mol×K	828.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R614209&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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