CADALA-1(10),3,8-TRIENE

Inchi: InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5-8,10-11,13,15H,9H2,1
InchiKey: GHOAKWKHPKLCNK-UHFFFAOYSA-N
Formula: C15H22
SMILES: CC1=C2C=CC(C)CC2C(C(C)C)C=C1
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
hfus	22.91	kJ/mol	Joback Method
logp	4.357		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
rinpol	1562.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.31	J/mol×K	575.49	Joback Method
cpg	595.19	J/mol×K	792.92	Joback Method
cpg	579.43	J/mol×K	756.68	Joback Method
cpg	562.58	J/mol×K	720.45	Joback Method
cpg	544.60	J/mol×K	684.21	Joback Method
cpg	525.43	J/mol×K	647.97	Joback Method
cpg	505.01	J/mol×K	611.73	Joback Method
dvisc	0.0005973	Pa×s	432.09	Joback Method
dvisc	0.0003464	Pa×s	575.49	Joback Method
dvisc	0.0004019	Pa×s	527.69	Joback Method
dvisc	0.0004804	Pa×s	479.89	Joback Method
dvisc	0.0017701	Pa×s	288.69	Joback Method
dvisc	0.0007840	Pa×s	384.29	Joback Method
dvisc	0.0011118	Pa×s	336.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U140056&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices