

Muurola-4,10(14)-dien-1«beta»-ol

Inchi:	InChI=1S/C15H24O/c1-10(2)13-6-5-12(4)15(16)8-7-11(3)9-14(13)15/h9-10,13-14,16H,4-
InchiKey:	URABJKMBRKSXSG-ZHDDOTHNSA-N
Formula:	C15H24O
SMILES:	C=C1CCC(C(C)C)C2C=C(C)CCC12O
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	17.49	kJ/mol	Joback Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1625.00		NIST Webbook
rinpol	1620.00		NIST Webbook
ripol	2177.00		NIST Webbook
ripol	2154.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.06	J/mol×K	663.77	Joback Method
cpg	590.64	J/mol×K	698.22	Joback Method
cpg	608.29	J/mol×K	732.68	Joback Method
cpg	625.13	J/mol×K	767.13	Joback Method
cpg	641.29	J/mol×K	801.59	Joback Method
cpg	656.87	J/mol×K	836.04	Joback Method
cpg	671.99	J/mol×K	870.50	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229440&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

Legend

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

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