«delta»-muurolene

Inchi: InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h9-10,13-15H,4-8H2,1-3
InchiKey: WRHGORWNJGOVQY-NFOMZHRRSA-N
Formula: C15H24
SMILES: C=C1CCC(C(C)C)C2C=C(C)CCC12
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	211.78	kJ/mol	Joback Method
hf	-127.04	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	49.91	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1467.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1681.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook
tb	571.35	K	Joback Method
tc	785.53	K	Joback Method
tf	288.33	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	501.64	J/mol×K	571.35	Joback Method
cpg	524.63	J/mol×K	607.05	Joback Method
cpg	546.31	J/mol×K	642.74	Joback Method
cpg	566.71	J/mol×K	678.44	Joback Method
cpg	585.88	J/mol×K	714.14	Joback Method
cpg	603.88	J/mol×K	749.83	Joback Method
cpg	620.74	J/mol×K	785.53	Joback Method
dvisc	0.0022043	Pa×s	288.33	Joback Method
dvisc	0.0013305	Pa×s	335.50	Joback Method
dvisc	0.0009095	Pa×s	382.67	Joback Method
dvisc	0.0006759	Pa×s	429.84	Joback Method
dvisc	0.0005326	Pa×s	477.01	Joback Method
dvisc	0.0004381	Pa×s	524.18	Joback Method
dvisc	0.0003722	Pa×s	571.35	Joback Method

Sources

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=R44932&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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