«alpha»-bisabol-1-one

Inchi: InChI=1S/C15H24O/c1-11(2)6-5-7-13(4)14-9-8-12(3)10-15(14)16/h6,10,13-14H,5,7-9H2,
InchiKey: KNOUERLLBMJGLF-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC(C)=CCCC(C)C1CCC(C)=CC1=O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	22.15	kJ/mol	Joback Method
ie	8.65	eV	Cheméo Relay (1.0)
logp	4.294		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
rinpol	1757.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1713.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.22	J/mol×K	637.71	Joback Method
cpg	575.88	J/mol×K	673.71	Joback Method
cpg	595.37	J/mol×K	709.70	Joback Method
cpg	613.70	J/mol×K	745.70	Joback Method
cpg	630.91	J/mol×K	781.70	Joback Method
cpg	647.03	J/mol×K	817.69	Joback Method
cpg	662.08	J/mol×K	853.69	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233444&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

Legend

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