

«beta»-Elemol

Inchi:	InChI=1S/C15H26O/c1-7-15(6)9-8-12(14(4,5)16)10-13(15)11(2)3/h7,12-13,16H,1-2,8-10
InchiKey:	GFJIQNADMLPFOW-GUTXKFCHSA-N
Formula:	C15H26O
SMILES:	<chem>C=CC1(C)CCC(C(C)(C)O)CC1C(=C)C</chem>
Mol. weight [g/mol]:	222.37
CAS:	32142-08-8

Physical Properties

Property code	Value	Unit	Source
gf	112.11	kJ/mol	Joback Method
hf	-243.96	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	61.77	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.942		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1536.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2069.00		NIST Webbook

ripol	2091.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2091.00		NIST Webbook
ripol	2105.00		NIST Webbook
tb	635.24	K	Joback Method
tc	836.45	K	Joback Method
tf	327.37	K	Joback Method
vc	0.775	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.75	J/mol×K	635.24	Joback Method
cpg	607.17	J/mol×K	668.78	Joback Method
cpg	625.55	J/mol×K	702.31	Joback Method
cpg	642.99	J/mol×K	735.85	Joback Method
cpg	659.62	J/mol×K	769.38	Joback Method
cpg	675.56	J/mol×K	802.92	Joback Method
cpg	690.93	J/mol×K	836.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32142088&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

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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