trans-2-Caren-4-ol

Other names:	E-2-Caren-4-ol
Inchi:	InChI=1S/C10H16O/c1-6-4-7-8(5-9(6)11)10(7,2)3/h4,7-9,11H,5H2,1-3H3
InchiKey:	XCIZLAMMPDJKRZ-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=CC2C(CC1O)C2(C)C
Mol. weight [g/mol]:	152.23
CAS:	4017-82-7

Physical Properties

Property code	Value	Unit	Source
gf	5.32	kJ/mol	Joback Method
hf	-241.65	kJ/mol	Joback Method
hfus	16.59	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1222.00		NIST Webbook
rinpol	1153.61		NIST Webbook
rinpol	1178.00		NIST Webbook
ripol	1816.00		NIST Webbook
tb	533.17	K	Joback Method
tc	729.30	K	Joback Method
tf	324.34	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.85	J/mol×K	533.17	Joback Method
cpg	351.53	J/mol×K	565.86	Joback Method
cpg	365.30	J/mol×K	598.55	Joback Method
cpg	378.26	J/mol×K	631.23	Joback Method

cpg	390.53	J/mol×K	663.92	Joback Method
cpg	402.21	J/mol×K	696.61	Joback Method
cpg	413.40	J/mol×K	729.30	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=C4017827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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