trans-«alpha»-Necrodol

Inchi: InChI=1S/C10H18O/c1-7-5-9(6-11)10(3,4)8(7)2/h5,8-9,11H,6H2,1-4H3/t8-,9+/m1/s1
InchiKey: KMSIDXMGNKQFNQ-BDAKNGLRSA-N
Formula: C10H18O
SMILES: CC1=CC(CO)C(C)(C)C1C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-67.53	kJ/mol	Joback Method
hf	-320.61	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	53.97	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.217		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1135.00		NIST Webbook
tb	530.70	K	Joback Method
tc	719.81	K	Joback Method
tf	302.88	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.43	J/mol×K	530.70	Joback Method
cpg	366.15	J/mol×K	562.22	Joback Method
cpg	380.10	J/mol×K	593.74	Joback Method
cpg	393.37	J/mol×K	625.25	Joback Method
cpg	406.02	J/mol×K	656.77	Joback Method
cpg	418.12	J/mol×K	688.29	Joback Method
cpg	429.75	J/mol×K	719.81	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R342271&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume