Galaxolide-I

Inchi: InChI=1S/C18H26O/c1-11-9-19-10-13-7-15-16(8-14(11)13)18(5,6)12(2)17(15,3)4/h7-8,1
InchiKey: ONKNPOPIGWHAQC-PIJUOVFKSA-N
Formula: C18H26O
SMILES: CC1COCc2cc3c(cc21)C(C)(C)C(C)C3(C)C
Mol. weight [g/mol]: 258.40

Physical Properties

Property code	Value	Unit	Source
gf	181.08	kJ/mol	Joback Method
hf	-215.49	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	61.51	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.525		Crippen Method
mcvol	224.870	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
ripol	2345.00		NIST Webbook
ripol	2345.00		NIST Webbook
tb	688.70	K	Joback Method
tc	920.33	K	Joback Method
tf	454.85	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.21	J/mol×K	688.70	Joback Method
cpg	681.77	J/mol×K	727.30	Joback Method
cpg	702.55	J/mol×K	765.91	Joback Method
cpg	722.86	J/mol×K	804.51	Joback Method
cpg	742.99	J/mol×K	843.12	Joback Method
cpg	763.23	J/mol×K	881.72	Joback Method
cpg	783.89	J/mol×K	920.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R631011&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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