o-xylene geranium

Inchi: InChI=1S/C18H26/c1-14(2)7-6-8-15(3)9-11-18-12-10-16(4)17(5)13-18/h7,9-10,12-13H,6,
InchiKey: IXKLZDQUHVBMOI-OQLLNIDSSA-N
Formula: C18H26
SMILES: CC(C)=CCCC(C)=CCc1ccc(C)c(C)c1
Mol. weight [g/mol]: 242.40

Physical Properties

Property code	Value	Unit	Source
gf	337.17	kJ/mol	Joback Method
hf	13.60	kJ/mol	Joback Method
hfus	33.42	kJ/mol	Joback Method
hvap	59.34	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.539		Crippen Method
mcvol	232.120	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	818.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	818.00		NIST Webbook
tb	655.96	K	Joback Method
tc	863.25	K	Joback Method
tf	306.00	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.31	J/mol×K	655.96	Joback Method
cpg	630.41	J/mol×K	690.51	Joback Method
cpg	648.43	J/mol×K	725.06	Joback Method
cpg	665.45	J/mol×K	759.60	Joback Method
cpg	681.53	J/mol×K	794.15	Joback Method
cpg	696.74	J/mol×K	828.70	Joback Method
cpg	711.15	J/mol×K	863.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R512539&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume