(E)-3,7-dimethylocta-2,6-dienyl anthranilate

Other names: Geranyl anthranilate
Inchi: InChI=1S/C17H23NO2/c1-13(2)7-6-8-14(3)11-12-20-17(19)15-9-4-5-10-16(15)18/h4-5,7,
InchiKey: QLRICECRKJGSKQ-SDNWHVSQSA-N
Formula: C17H23NO2
SMILES: CC(C)=CCCC(C)=CCOC(=O)c1ccccc1N
Mol. weight [g/mol]: 273.37
CAS: 67874-69-5

Physical Properties

Property code	Value	Unit	Source
gf	170.91	kJ/mol	Joback Method
hf	-165.30	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	76.25	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.118		Crippen Method
mcvol	235.450	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	2244.80		NIST Webbook
rinpol	2244.80		NIST Webbook
tb	776.92	K	Joback Method
tc	997.01	K	Joback Method
tf	437.63	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.99	J/mol×K	776.92	Joback Method
cpg	690.71	J/mol×K	813.60	Joback Method
cpg	705.43	J/mol×K	850.28	Joback Method
cpg	719.21	J/mol×K	886.97	Joback Method
cpg	732.14	J/mol×K	923.65	Joback Method
cpg	744.28	J/mol×K	960.33	Joback Method

cpg	755.69	J/mol×K	997.01	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=C67874695&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