Eugenyl anthranilate

Inchi: InChI=1S/C17H17NO3/c1-3-6-12-9-10-15(16(11-12)20-2)21-17(19)13-7-4-5-8-14(13)18/h
InchiKey: KFYPXGAXXLQPBI-UHFFFAOYSA-N
Formula: C17H17NO3
SMILES: C=CCc1ccc(OC(=O)c2ccccc2N)c(OC)c1
Mol. weight [g/mol]: 283.32
CAS: 861571-50-8

Physical Properties

Property code	Value	Unit	Source
gf	103.56	kJ/mol	Joback Method
hf	-173.36	kJ/mol	Joback Method
hfus	34.59	kJ/mol	Joback Method
hvap	81.51	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.225		Crippen Method
mcvol	221.860	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	2437.80		NIST Webbook
rinpol	2437.80		NIST Webbook
tb	824.58	K	Joback Method
tc	1061.77	K	Joback Method
tf	547.64	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.70	J/mol×K	824.58	Joback Method
cpg	646.23	J/mol×K	864.11	Joback Method
cpg	658.55	J/mol×K	903.64	Joback Method
cpg	669.69	J/mol×K	943.18	Joback Method
cpg	679.67	J/mol×K	982.71	Joback Method
cpg	688.53	J/mol×K	1022.24	Joback Method
cpg	696.28	J/mol×K	1061.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C861571508&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