Kebuzone, methylated

Inchi: InChI=1S/C22H22O3/c1-15(23)13-14-18-21(24)19(16-9-5-3-6-10-16)20(22(18)25-2)17-1
InchiKey: SYNIYGVOSYJTFL-UHFFFAOYSA-N
Formula: C22H22O3
SMILES: COC1=C(c2ccccc2)C(c2ccccc2)C(=O)C1CCC(C)=O
Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	42.21	kJ/mol	Joback Method
hf	-331.87	kJ/mol	Joback Method
hfus	38.56	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.396		Crippen Method
mcvol	267.170	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2510.00		NIST Webbook
tb	919.96	K	Joback Method
tc	1167.45	K	Joback Method
tf	563.38	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.80	J/mol×K	919.96	Joback Method
cpg	863.92	J/mol×K	961.21	Joback Method
cpg	877.25	J/mol×K	1002.46	Joback Method
cpg	888.83	J/mol×K	1043.70	Joback Method
cpg	898.69	J/mol×K	1084.95	Joback Method
cpg	906.88	J/mol×K	1126.20	Joback Method
cpg	913.43	J/mol×K	1167.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201719&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