Eugenol, «beta»-D-glucopyranoside, TFA

Other names: Eugenol, Gly, TFA
Inchi: InChI=1S/C24H18F12O11/c1-3-4-9-5-6-10(11(7-9)41-2)43-16-15(47-20(40)24(34,35)36)
InchiKey: OXPQPWKLKWTOPR-QMHWVQJVSA-N
Formula: C24H18F12O11
SMILES: C=CCc1ccc(OC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC(=
Mol. weight [g/mol]: 710.37

Physical Properties

Property code	Value	Unit	Source
gf	-3232.36	kJ/mol	Joback Method
hf	-3990.67	kJ/mol	Joback Method
hfus	74.83	kJ/mol	Joback Method
hvap	102.11	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.055		Crippen Method
mcvol	378.710	ml/mol	McGowan Method
pc	850.48	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2039.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2039.00		NIST Webbook
tb	1137.98	K	Joback Method
tc	1429.86	K	Joback Method
tf	776.79	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.17	J/mol×K	1137.98	Joback Method
cpg	1321.83	J/mol×K	1186.63	Joback Method
cpg	1321.30	J/mol×K	1235.27	Joback Method
cpg	1317.69	J/mol×K	1283.92	Joback Method

cpg	1311.10	J/mol×K	1332.57	Joback Method
cpg	1301.63	J/mol×K	1381.21	Joback Method
cpg	1289.37	J/mol×K	1429.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184788&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