Citronellol, Gly, TFA

Inchi: InChI=1S/C24H26F12O10/c1-10(2)5-4-6-11(3)7-8-41-16-15(46-20(40)24(34,35)36)14(45
InchiKey: ZJAHYNJNLFTXKW-YTQIUSBHSA-N
Formula: C24H26F12O10
SMILES: CC(C)=CCCC(C)CCOC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C
Mol. weight [g/mol]: 702.44

Physical Properties

Property code	Value	Unit	Source
gf	-3239.12	kJ/mol	Joback Method
hf	-4095.32	kJ/mol	Joback Method
hfus	77.02	kJ/mol	Joback Method
hvap	96.42	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.028		Crippen Method
mcvol	396.600	ml/mol	McGowan Method
pc	734.42	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	1085.84	K	Joback Method
tc	1373.56	K	Joback Method
tf	670.82	K	Joback Method
vc	1.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1424.08	J/mol×K	1085.84	Joback Method
cpg	1434.65	J/mol×K	1133.79	Joback Method
cpg	1442.46	J/mol×K	1181.75	Joback Method
cpg	1447.67	J/mol×K	1229.70	Joback Method
cpg	1450.46	J/mol×K	1277.65	Joback Method
cpg	1451.00	J/mol×K	1325.61	Joback Method
cpg	1449.45	J/mol×K	1373.56	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=R394673&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