Esfenvalerate, isomer 2

Inchi: InChI=1S/C25H22ClNO3/c1-17(2)24(19-8-12-20(26)13-9-19)25(28)30-23(16-27)18-10-14
InchiKey: MKLAMBQQMOQHPH-UHFFFAOYSA-N
Formula: C25H22ClNO3
SMILES: CC(C)C(C(=O)OC(C#N)c1ccc(Oc2ccccc2)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]: 419.90

Physical Properties

Property code	Value	Unit	Source
gf	252.60	kJ/mol	Joback Method
hf	-116.40	kJ/mol	Joback Method
hfus	40.96	kJ/mol	Joback Method
hvap	104.66	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.680		Crippen Method
mcvol	318.760	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	2982.00		NIST Webbook
rinpol	2982.00		NIST Webbook
tb	1098.30	K	Joback Method
tc	1359.75	K	Joback Method
tf	620.11	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.65	J/mol×K	1098.30	Joback Method
cpg	994.49	J/mol×K	1141.87	Joback Method
cpg	1001.88	J/mol×K	1185.45	Joback Method
cpg	1007.90	J/mol×K	1229.02	Joback Method
cpg	1012.66	J/mol×K	1272.60	Joback Method
cpg	1016.26	J/mol×K	1316.17	Joback Method
cpg	1018.78	J/mol×K	1359.75	Joback Method

Sources

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=R566482&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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