o-Allyl oo-tert-butylperfumarate

Inchi: InChI=1S/C11H16O5/c1-5-8-14-9(12)6-7-10(13)15-16-11(2,3)4/h5-7H,1,8H2,2-4H3/b7-6
InchiKey: ZPVRKKIWIZMFSM-VOTSOKGWSA-N
Formula: C11H16O5
SMILES: C=CCOC(=O)C=CC(=O)OOC(C)(C)C
Mol. weight [g/mol]: 228.24
CAS: 52345-51-4

Physical Properties

Property code	Value	Unit	Source
gf	-360.20	kJ/mol	Joback Method
hf	-658.29	kJ/mol	Joback Method
hfl	-673.20 ± 4.20	kJ/mol	NIST Webbook
hfus	22.52	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.545		Crippen Method
mcvol	178.000	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
tb	623.69	K	Joback Method
tc	820.57	K	Joback Method
tf	375.86	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.07	J/mol×K	623.69	Joback Method
cpg	465.27	J/mol×K	656.50	Joback Method
cpg	477.73	J/mol×K	689.32	Joback Method
cpg	489.49	J/mol×K	722.13	Joback Method
cpg	500.55	J/mol×K	754.94	Joback Method
cpg	510.93	J/mol×K	787.76	Joback Method
cpg	520.64	J/mol×K	820.57	Joback Method
dvisc	0.0012633	Pa×s	375.86	Joback Method

dvisc	0.0006791	Pa×s	417.17	Joback Method
dvisc	0.0004082	Pa×s	458.47	Joback Method
dvisc	0.0002669	Pa×s	499.78	Joback Method
dvisc	0.0001862	Pa×s	541.08	Joback Method
dvisc	0.0001368	Pa×s	582.38	Joback Method
dvisc	0.0001046	Pa×s	623.69	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=C52345514&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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