«alpha»-Kessyl hexanoate

Inchi: InChI=1S/C21H36O3/c1-6-7-8-9-19(22)23-18-13-21(5)16-11-10-14(2)15(16)12-17(18)20
InchiKey: MNBLJUIWDVQHEP-AYNZCFQGSA-N
Formula: C21H36O3
SMILES: CCCCCC(=O)OC1CC2(C)OC(C)(C)C1CC1C(C)CCC12
Mol. weight [g/mol]: 336.51

Physical Properties

Property code	Value	Unit	Source
gf	-89.97	kJ/mol	Joback Method
hf	-704.53	kJ/mol	Joback Method
hfus	40.70	kJ/mol	Joback Method
hvap	72.72	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.118		Crippen Method
mcvol	287.480	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2070.00		NIST Webbook
tb	797.95	K	Joback Method
tc	1009.51	K	Joback Method
tf	499.26	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.80	J/mol×K	797.95	Joback Method
cpg	1001.52	J/mol×K	833.21	Joback Method
cpg	1025.75	J/mol×K	868.47	Joback Method
cpg	1049.72	J/mol×K	903.73	Joback Method
cpg	1073.64	J/mol×K	938.99	Joback Method
cpg	1097.76	J/mol×K	974.25	Joback Method
cpg	1122.29	J/mol×K	1009.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224792&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