1-ethyl-2-methylpropyl 3,13-dimethylpentadecanoate

Inchi: InChI=1S/C23H46O2/c1-7-20(5)16-14-12-10-9-11-13-15-17-21(6)18-23(24)25-22(8-2)19
InchiKey: AJQJSPMMDNUUDH-UHFFFAOYSA-N
Formula: C23H46O2
SMILES: CCC(C)CCCCCCCCCC(C)CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 354.61

Physical Properties

Property code	Value	Unit	Source
gf	-100.90	kJ/mol	Joback Method
hf	-783.97	kJ/mol	Joback Method
hfus	44.02	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.547		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	892.13	kPa	Joback Method
rinpol	2279.00		NIST Webbook
tb	800.17	K	Joback Method
tc	982.73	K	Joback Method
tf	361.13	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.26	J/mol×K	800.17	Joback Method
cpg	1116.64	J/mol×K	830.60	Joback Method
cpg	1136.87	J/mol×K	861.02	Joback Method
cpg	1155.98	J/mol×K	891.45	Joback Method
cpg	1174.02	J/mol×K	921.87	Joback Method
cpg	1191.00	J/mol×K	952.30	Joback Method
cpg	1206.97	J/mol×K	982.73	Joback Method
dvisc	0.0032612	Pa×s	361.13	Joback Method
dvisc	0.0008061	Pa×s	434.30	Joback Method

dvisc	0.0002982	Pa×s	507.48	Joback Method
dvisc	0.0001417	Pa×s	580.65	Joback Method
dvisc	0.0000795	Pa×s	653.82	Joback Method
dvisc	0.0000502	Pa×s	727.00	Joback Method
dvisc	0.0000344	Pa×s	800.17	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=R422778&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
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