10,14-Dimethylpentadecyl isobutyrate

Inchi: InChI=1S/C21H42O2/c1-18(2)14-13-16-20(5)15-11-9-7-6-8-10-12-17-23-21(22)19(3)4/h1
InchiKey: WEUUVFYXSHQOIT-UHFFFAOYSA-N
Formula: C21H42O2
SMILES: CC(C)CCCC(C)CCCCCCCCCCOC(=O)C(C)C
Mol. weight [g/mol]: 326.56

Physical Properties

Property code	Value	Unit	Source
gf	-115.30	kJ/mol	Joback Method
hf	-737.41	kJ/mol	Joback Method
hfus	42.36	kJ/mol	Joback Method
hvap	70.33	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	6.769		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	998.91	kPa	Joback Method
rinpol	2147.00		NIST Webbook
tb	754.85	K	Joback Method
tc	931.67	K	Joback Method
tf	353.59	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.62	J/mol×K	754.85	Joback Method
cpg	1063.27	J/mol×K	902.20	Joback Method
cpg	1046.69	J/mol×K	872.73	Joback Method
cpg	1029.16	J/mol×K	843.26	Joback Method
cpg	1010.65	J/mol×K	813.79	Joback Method
cpg	991.15	J/mol×K	784.32	Joback Method
cpg	1078.94	J/mol×K	931.67	Joback Method
dvisc	0.0000501	Pa×s	754.85	Joback Method
dvisc	0.0000715	Pa×s	687.97	Joback Method

dvisc	0.0001103	Pa×s	621.10	Joback Method
dvisc	0.0001889	Pa×s	554.22	Joback Method
dvisc	0.0003751	Pa×s	487.34	Joback Method
dvisc	0.0009261	Pa×s	420.47	Joback Method
dvisc	0.0032188	Pa×s	353.59	Joback Method

Sources

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=R422783&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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