ethyl 13-(cyclopent-2-enyl)tridecanoate

Other names: 2-Cyclopentene-1-tridecanoic acid, ethyl ester, (S)-
Inchi: InChI=1S/C20H36O2/c1-2-22-20(21)18-12-10-8-6-4-3-5-7-9-11-15-19-16-13-14-17-19/h1
InchiKey: FDGHZUQYDACRTA-IBGZPJMESA-N
Formula: C20H36O2
SMILES: CCOC(=O)CCCCCCCCCCCCC1C=CCC1
Mol. weight [g/mol]: 308.50
CAS: 623-32-5

Physical Properties

Property code	Value	Unit	Source
gf	-49.89	kJ/mol	Joback Method
hf	-582.67	kJ/mol	Joback Method
hfus	45.50	kJ/mol	Joback Method
hvap	69.82	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.197		Crippen Method
mcvol	284.940	ml/mol	McGowan Method
pc	1208.99	kPa	Joback Method
rinpol	2256.50		NIST Webbook
rinpol	2256.50		NIST Webbook
tb	747.73	K	Joback Method
tc	931.67	K	Joback Method
tf	398.98	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.62	J/mol×K	747.73	Joback Method
cpg	965.68	J/mol×K	901.01	Joback Method
cpg	949.85	J/mol×K	870.35	Joback Method
cpg	933.07	J/mol×K	839.70	Joback Method
cpg	915.29	J/mol×K	809.04	Joback Method
cpg	896.49	J/mol×K	778.39	Joback Method

cpg	980.58	J/mol×K	931.67	Joback Method
dvisc	0.0001137	Pa×s	747.73	Joback Method
dvisc	0.0001486	Pa×s	689.61	Joback Method
dvisc	0.0002041	Pa×s	631.48	Joback Method
dvisc	0.0002989	Pa×s	573.36	Joback Method
dvisc	0.0004772	Pa×s	515.23	Joback Method
dvisc	0.0008579	Pa×s	457.10	Joback Method
dvisc	0.0018300	Pa×s	398.98	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	503.20	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C623325&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume