Sebacic acid, ethyl 3-methylpentyl ester

Inchi: InChI=1S/C18H34O4/c1-4-16(3)14-15-22-18(20)13-11-9-7-6-8-10-12-17(19)21-5-2/h16H
InchiKey: BQCSOYIPJOCULF-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCOC(=O)CCCCCCCCC(=O)OCCC(C)CC
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-369.60	kJ/mol	Joback Method
hf	-909.73	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.650		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinpol	2168.00		NIST Webbook
tb	763.38	K	Joback Method
tc	943.41	K	Joback Method
tf	421.94	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.98	J/mol×K	763.38	Joback Method
cpg	867.53	J/mol×K	793.39	Joback Method
cpg	884.14	J/mol×K	823.39	Joback Method
cpg	899.82	J/mol×K	853.40	Joback Method
cpg	914.60	J/mol×K	883.40	Joback Method
cpg	928.46	J/mol×K	913.41	Joback Method
cpg	941.44	J/mol×K	943.41	Joback Method
dvisc	0.0012393	Pa×s	421.94	Joback Method
dvisc	0.0005664	Pa×s	478.85	Joback Method

dvisc	0.0003058	Pa×s	535.75	Joback Method
dvisc	0.0001858	Pa×s	592.66	Joback Method
dvisc	0.0001232	Pa×s	649.57	Joback Method
dvisc	0.0000873	Pa×s	706.47	Joback Method
dvisc	0.0000651	Pa×s	763.38	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=U355612&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