Sebacic acid, isobutyl pent-4-en-2-yl ester

Inchi: InChI=1S/C19H34O4/c1-5-12-17(4)23-19(21)14-11-9-7-6-8-10-13-18(20)22-15-16(2)3/h5
InchiKey: IRACLSLDWMQWFK-UHFFFAOYSA-N
Formula: C19H34O4
SMILES: C=CCC(C)OC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-275.78	kJ/mol	Joback Method
hf	-810.22	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	74.75	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.814		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	782.50	K	Joback Method
tc	966.47	K	Joback Method
tf	416.45	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.50	J/mol×K	782.50	Joback Method
cpg	901.04	J/mol×K	813.16	Joback Method
cpg	917.59	J/mol×K	843.82	Joback Method
cpg	933.16	J/mol×K	874.48	Joback Method
cpg	947.78	J/mol×K	905.15	Joback Method
cpg	961.47	J/mol×K	935.81	Joback Method
cpg	974.23	J/mol×K	966.47	Joback Method
dvisc	0.0013543	Pa×s	416.45	Joback Method

dvisc	0.0005655	Pa×s	477.46	Joback Method
dvisc	0.0002878	Pa×s	538.47	Joback Method
dvisc	0.0001680	Pa×s	599.48	Joback Method
dvisc	0.0001084	Pa×s	660.48	Joback Method
dvisc	0.0000753	Pa×s	721.49	Joback Method
dvisc	0.0000553	Pa×s	782.50	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=U355950&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