Sebacic acid, but-3-enyl undecyl ester

Inchi: InChI=1S/C25H46O4/c1-3-5-7-8-9-10-13-16-19-23-29-25(27)21-18-15-12-11-14-17-20-2
InchiKey: INWUROFBHOQUNK-UHFFFAOYSA-N
Formula: C25H46O4
SMILES: C=CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-220.38	kJ/mol	Joback Method
hf	-923.50	kJ/mol	Joback Method
hfus	64.80	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.300		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	823.84	kPa	Joback Method
rinpol	2862.00		NIST Webbook
tb	920.66	K	Joback Method
tc	1129.75	K	Joback Method
tf	514.07	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.87	J/mol×K	920.66	Joback Method
cpg	1338.57	J/mol×K	1094.90	Joback Method
cpg	1323.94	J/mol×K	1060.05	Joback Method
cpg	1308.00	J/mol×K	1025.21	Joback Method
cpg	1290.71	J/mol×K	990.36	Joback Method
cpg	1272.01	J/mol×K	955.51	Joback Method
cpg	1351.93	J/mol×K	1129.75	Joback Method
dvisc	0.0000272	Pa×s	920.66	Joback Method
dvisc	0.0000362	Pa×s	852.89	Joback Method

dvisc	0.0000508	Pa×s	785.13	Joback Method
dvisc	0.0000759	Pa×s	717.37	Joback Method
dvisc	0.0001233	Pa×s	649.60	Joback Method
dvisc	0.0002242	Pa×s	581.84	Joback Method
dvisc	0.0004774	Pa×s	514.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356091&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume