Sebacic acid, but-3-enyl octyl ester

Inchi: InChI=1S/C22H40O4/c1-3-5-7-8-13-16-20-26-22(24)18-15-12-10-9-11-14-17-21(23)25-1
InchiKey: ZVTMFHJASTZZKZ-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: C=CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-245.64	kJ/mol	Joback Method
hf	-861.58	kJ/mol	Joback Method
hfus	57.03	kJ/mol	Joback Method
hvap	82.21	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.130		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	979.01	kPa	Joback Method
rinpol	2567.00		NIST Webbook
tb	852.02	K	Joback Method
tc	1043.34	K	Joback Method
tf	480.26	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.09	J/mol×K	852.02	Joback Method
cpg	1145.82	J/mol×K	1011.45	Joback Method
cpg	1131.66	J/mol×K	979.56	Joback Method
cpg	1116.44	J/mol×K	947.68	Joback Method
cpg	1100.12	J/mol×K	915.79	Joback Method
cpg	1082.68	J/mol×K	883.91	Joback Method
cpg	1158.94	J/mol×K	1043.34	Joback Method
dvisc	0.0000426	Pa×s	852.02	Joback Method
dvisc	0.0000564	Pa×s	790.06	Joback Method

dvisc	0.0000784	Pa×s	728.10	Joback Method
dvisc	0.0001158	Pa×s	666.14	Joback Method
dvisc	0.0001853	Pa×s	604.18	Joback Method
dvisc	0.0003301	Pa×s	542.22	Joback Method
dvisc	0.0006825	Pa×s	480.26	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=U356088&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