Sebacic acid, 3-methylbut-2-enyl nonyl ester

Inchi: InChI=1S/C24H44O4/c1-4-5-6-7-10-13-16-20-27-23(25)17-14-11-8-9-12-15-18-24(26)28
InchiKey: YYKBBJWZNHUKIB-UHFFFAOYSA-N
Formula: C24H44O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-244.97	kJ/mol	Joback Method
hf	-920.86	kJ/mol	Joback Method
hfus	62.38	kJ/mol	Joback Method
hvap	87.37	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.910		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	878.96	kPa	Joback Method
rinpol	2787.00		NIST Webbook
tb	905.14	K	Joback Method
tc	1108.46	K	Joback Method
tf	485.52	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.16	J/mol×K	905.14	Joback Method
cpg	1209.71	J/mol×K	939.03	Joback Method
cpg	1227.98	J/mol×K	972.91	Joback Method
cpg	1245.02	J/mol×K	1006.80	Joback Method
cpg	1260.87	J/mol×K	1040.69	Joback Method
cpg	1275.58	J/mol×K	1074.58	Joback Method
cpg	1289.20	J/mol×K	1108.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355882&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
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