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

Inchi: InChI=1S/C26H48O4/c1-4-5-6-7-8-9-12-15-18-22-29-25(27)19-16-13-10-11-14-17-20-26
InchiKey: UZFCIOJYLVFSHX-UHFFFAOYSA-N
Formula: C26H48O4
SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-228.13	kJ/mol	Joback Method
hf	-962.14	kJ/mol	Joback Method
hfus	67.56	kJ/mol	Joback Method
hvap	91.82	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.691		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	786.83	kPa	Joback Method
rinpol	2992.00		NIST Webbook
tb	950.90	K	Joback Method
tc	1168.20	K	Joback Method
tf	508.06	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.19	J/mol×K	950.90	Joback Method
cpg	1337.88	J/mol×K	987.12	Joback Method
cpg	1357.08	J/mol×K	1023.33	Joback Method
cpg	1374.86	J/mol×K	1059.55	Joback Method
cpg	1391.28	J/mol×K	1095.77	Joback Method
cpg	1406.39	J/mol×K	1131.98	Joback Method
cpg	1420.28	J/mol×K	1168.20	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355884&Units=SI

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