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

Inchi: InChI=1S/C25H46O4/c1-4-5-6-7-8-11-14-17-21-28-24(26)18-15-12-9-10-13-16-19-25(27
InchiKey: XBMDYCYGVXXIDH-UHFFFAOYSA-N
Formula: C25H46O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-236.55	kJ/mol	Joback Method
hf	-941.50	kJ/mol	Joback Method
hfus	64.97	kJ/mol	Joback Method
hvap	89.59	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.300		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	830.98	kPa	Joback Method
rinpol	2889.00		NIST Webbook
rinpol	2889.00		NIST Webbook
tb	928.02	K	Joback Method
tc	1137.79	K	Joback Method
tf	496.79	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.42	J/mol×K	928.02	Joback Method
cpg	1273.51	J/mol×K	962.98	Joback Method
cpg	1292.23	J/mol×K	997.94	Joback Method
cpg	1309.62	J/mol×K	1032.90	Joback Method
cpg	1325.75	J/mol×K	1067.86	Joback Method
cpg	1340.66	J/mol×K	1102.83	Joback Method
cpg	1354.42	J/mol×K	1137.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355883&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