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

Inchi: InChI=1S/C27H50O4/c1-4-5-6-7-8-9-10-13-16-19-23-30-26(28)20-17-14-11-12-15-18-21
InchiKey: CDIRWXSCWFTRTI-UHFFFAOYSA-N
Formula: C27H50O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-219.71	kJ/mol	Joback Method
hf	-982.78	kJ/mol	Joback Method
hfus	70.15	kJ/mol	Joback Method
hvap	94.05	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.081		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	746.11	kPa	Joback Method
rinpol	3095.00		NIST Webbook
tb	973.78	K	Joback Method
tc	1199.79	K	Joback Method
tf	519.33	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.44	J/mol×K	973.78	Joback Method
cpg	1402.78	J/mol×K	1011.45	Joback Method
cpg	1422.50	J/mol×K	1049.12	Joback Method
cpg	1440.69	J/mol×K	1086.79	Joback Method
cpg	1457.41	J/mol×K	1124.46	Joback Method
cpg	1472.73	J/mol×K	1162.13	Joback Method
cpg	1486.74	J/mol×K	1199.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355885&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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