Sebacic acid, 3-heptyl octyl ester

Inchi: InChI=1S/C25H48O4/c1-4-7-9-10-15-18-22-28-24(26)20-16-13-11-12-14-17-21-25(27)29
InchiKey: PIFFUSBQTLDZRH-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)CCCC
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-310.66	kJ/mol	Joback Method
hf	-1054.21	kJ/mol	Joback Method
hfus	62.56	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.523		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
rinpol	2771.00		NIST Webbook
rinpol	2771.00		NIST Webbook
tb	923.54	K	Joback Method
tc	1133.47	K	Joback Method
tf	500.83	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.56	J/mol×K	923.54	Joback Method
cpg	1369.84	J/mol×K	1098.48	Joback Method
cpg	1355.09	J/mol×K	1063.49	Joback Method
cpg	1338.92	J/mol×K	1028.50	Joback Method
cpg	1321.30	J/mol×K	993.52	Joback Method
cpg	1302.20	J/mol×K	958.53	Joback Method
cpg	1383.23	J/mol×K	1133.47	Joback Method
dvisc	0.0000230	Pa×s	923.54	Joback Method

dvisc	0.0000313	Pa×s	853.09	Joback Method
dvisc	0.0000450	Pa×s	782.64	Joback Method
dvisc	0.0000695	Pa×s	712.18	Joback Method
dvisc	0.0001181	Pa×s	641.73	Joback Method
dvisc	0.0002287	Pa×s	571.28	Joback Method
dvisc	0.0005334	Pa×s	500.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355582&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
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

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