Decanedioic acid, dinonyl ester

Other names: Sebacic acid, dinonyl ester
dinonyl sebacate
Inchi: InChI=1S/C28H54O4/c1-3-5-7-9-13-17-21-25-31-27(29)23-19-15-11-12-16-20-24-28(30)
InchiKey: VNTXONBESJNLBI-UHFFFAOYSA-N
Formula: C28H54O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]: 454.73
CAS: 4121-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-282.96	kJ/mol	Joback Method
hf	-1110.85	kJ/mol	Joback Method
hfus	73.85	kJ/mol	Joback Method
hvap	96.23	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	8.695		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	687.45	kPa	Joback Method
rinpol	3234.00		NIST Webbook
rinpol	3234.00		NIST Webbook
tb	992.62	K	Joback Method
tc	1233.15	K	Joback Method
tf	549.64	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.57	J/mol×K	992.62	Joback Method
cpg	1497.33	J/mol×K	1032.71	Joback Method
cpg	1518.05	J/mol×K	1072.80	Joback Method
cpg	1536.79	J/mol×K	1112.88	Joback Method
cpg	1553.63	J/mol×K	1152.97	Joback Method

cpg	1568.65	J/mol×K	1193.06	Joback Method
cpg	1581.91	J/mol×K	1233.15	Joback Method
dvisc	0.0003138	Pa×s	549.64	Joback Method
dvisc	0.0001419	Pa×s	623.47	Joback Method
dvisc	0.0000759	Pa×s	697.30	Joback Method
dvisc	0.0000458	Pa×s	771.13	Joback Method
dvisc	0.0000302	Pa×s	844.96	Joback Method
dvisc	0.0000212	Pa×s	918.79	Joback Method
dvisc	0.0000158	Pa×s	992.62	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=C4121168&Units=SI

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