Decanedioic acid, diisooctyl ester

Other names: Sebacic acid, dioctyl ester
diisooctyl sebacate
Inchi: InChI=1S/C26H50O4/c1-23(2)17-11-9-15-21-29-25(27)19-13-7-5-6-8-14-20-26(28)30-22
InchiKey: ZWYAVGUHWPLBGT-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CC(C)CCCCCOC(=O)CCCCCCCCC(=O)OCCCCCC(C)C
Mol. weight [g/mol]: 426.67
CAS: 27214-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-304.68	kJ/mol	Joback Method
hf	-1080.13	kJ/mol	Joback Method
hfus	61.62	kJ/mol	Joback Method
hvap	91.01	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.626		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	769.04	kPa	Joback Method
rinpol	3033.00		NIST Webbook
rinpol	3033.00		NIST Webbook
tb	945.98	K	Joback Method
tc	1162.69	K	Joback Method
tf	497.10	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.96	J/mol×K	945.98	Joback Method
cpg	1367.00	J/mol×K	982.10	Joback Method
cpg	1386.38	J/mol×K	1018.22	Joback Method
cpg	1404.14	J/mol×K	1054.33	Joback Method
cpg	1420.33	J/mol×K	1090.45	Joback Method

cpg	1435.00	J/mol×K	1126.57	Joback Method
cpg	1448.19	J/mol×K	1162.69	Joback Method
dvisc	0.0005428	Pa×s	497.10	Joback Method
dvisc	0.0002121	Pa×s	571.91	Joback Method
dvisc	0.0001030	Pa×s	646.73	Joback Method
dvisc	0.0000581	Pa×s	721.54	Joback Method
dvisc	0.0000365	Pa×s	796.35	Joback Method
dvisc	0.0000248	Pa×s	871.17	Joback Method
dvisc	0.0000180	Pa×s	945.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27214900&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
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