Decanedioic acid, dioctyl ester

Other names:	Dioctyl sebacate
	decadioic acid, dioctyl ester
	Di-n-octyl sebacate
Inchi:	InChI=1S/C26H50O4/c1-3-5-7-9-15-19-23-29-25(27)21-17-13-11-12-14-18-22-26(28)30-
InchiKey:	MIMDHDXOBDPUQW-UHFFFAOYSA-N
Formula:	C26H50O4
SMILES:	CCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	426.67
CAS:	2432-87-3

Physical Properties

Property code	Value	Unit	Source
gf	-299.80	kJ/mol	Joback Method
hf	-1069.57	kJ/mol	Joback Method
hfus	68.67	kJ/mol	Joback Method
hvap	120.80 ± 4.20	kJ/mol	NIST Webbook
log10ws	-8.43		Crippen Method
logp	7.915		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	762.26	kPa	Joback Method
rinpol	458.80		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2778.00		NIST Webbook
rinpol	458.70		NIST Webbook
rinpol	2773.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	458.80		NIST Webbook
rinpol	2773.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	946.86	K	Joback Method
tc	1166.44	K	Joback Method
tf	527.10	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.23	J/mol×K	946.86	Joback Method
cpg	1435.85	J/mol×K	1129.84	Joback Method
cpg	1420.89	J/mol×K	1093.25	Joback Method
cpg	1404.40	J/mol×K	1056.65	Joback Method
cpg	1386.33	J/mol×K	1020.05	Joback Method
cpg	1366.62	J/mol×K	983.46	Joback Method
cpg	1449.33	J/mol×K	1166.44	Joback Method
cpl	849.00	J/mol×K	318.00	NIST Webbook
dvisc	0.0004085	Pa×s	527.10	Joback Method
dvisc	0.0000216	Pa×s	946.86	Joback Method
dvisc	0.0000290	Pa×s	876.90	Joback Method
dvisc	0.0000410	Pa×s	806.94	Joback Method
dvisc	0.0000618	Pa×s	736.98	Joback Method
dvisc	0.0001016	Pa×s	667.02	Joback Method
dvisc	0.0001878	Pa×s	597.06	Joback Method
hvapt	109.70	kJ/mol	368.00	NIST Webbook
hvapt	107.10	kJ/mol	468.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2432873&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
cpl: Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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