Decanedioic acid, dipentyl ester

Other names: dipentyl sebacate
Inchi: InChI=1S/C20H38O4/c1-3-5-13-17-23-19(21)15-11-9-7-8-10-12-16-20(22)24-18-14-6-4-2
InchiKey: WZURZWRVLHOHAS-UHFFFAOYSA-N
Formula: C20H38O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 342.51
CAS: 6819-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-350.32	kJ/mol	Joback Method
hf	-945.73	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.574		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1077.81	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	809.58	K	Joback Method
tc	993.33	K	Joback Method
tf	459.48	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.18	J/mol×K	809.58	Joback Method
cpg	987.44	J/mol×K	840.20	Joback Method
cpg	1004.65	J/mol×K	870.83	Joback Method
cpg	1020.84	J/mol×K	901.45	Joback Method
cpg	1036.02	J/mol×K	932.08	Joback Method
cpg	1050.21	J/mol×K	962.70	Joback Method

cpg	1063.43	J/mol×K	993.33	Joback Method
dvisc	0.0008397	Pa×s	459.48	Joback Method
dvisc	0.0004093	Pa×s	517.83	Joback Method
dvisc	0.0002308	Pa×s	576.18	Joback Method
dvisc	0.0001446	Pa×s	634.53	Joback Method
dvisc	0.0000980	Pa×s	692.88	Joback Method
dvisc	0.0000706	Pa×s	751.23	Joback Method
dvisc	0.0000533	Pa×s	809.58	Joback Method
hvapt	99.20	kJ/mol	380.50	NIST Webbook

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=C6819096&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
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

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