

Sebacic acid, tetrahydrofurfuryl pentyl ester

Inchi:	InChI=1S/C20H36O5/c1-2-3-10-15-24-19(21)13-8-6-4-5-7-9-14-20(22)25-17-18-12-11-16
InchiKey:	VCSINEZGWBIMLW-UHFFFAOYSA-N
Formula:	C20H36O5
SMILES:	CCCCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	356.50

Physical Properties

Property code	Value	Unit	Source
gf	-399.89	kJ/mol	Joback Method
hf	-1017.25	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	83.19	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.563		Crippen Method
mvol	302.550	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	2607.00		NIST Webbook
tb	851.81	K	Joback Method
tc	1047.64	K	Joback Method
tf	496.95	K	Joback Method
vc	1.165	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.21	J/molxK	851.81	Joback Method
cpg	1074.94	J/molxK	1015.00	Joback Method
cpg	1061.73	J/molxK	982.37	Joback Method
cpg	1047.38	J/molxK	949.73	Joback Method
cpg	1031.86	J/molxK	917.09	Joback Method
cpg	1015.15	J/molxK	884.45	Joback Method
cpg	1087.03	J/molxK	1047.64	Joback Method
dvisc	0.0000679	Paxs	851.81	Joback Method
dvisc	0.0000888	Paxs	792.67	Joback Method

dvisc	0.0001213	Paxs	733.52	Joback Method
dvisc	0.0001751	Paxs	674.38	Joback Method
dvisc	0.0002711	Paxs	615.24	Joback Method
dvisc	0.0004608	Paxs	556.09	Joback Method
dvisc	0.0008884	Paxs	496.95	Joback Method

Sources

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=U355721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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