

Sebacic acid, heptyl 2-methoxyethyl ester

Inchi:	InChI=1S/C20H38O5/c1-3-4-5-10-13-16-24-19(21)14-11-8-6-7-9-12-15-20(22)25-18-17-2
InchiKey:	FNCXXISHAIOOGE-UHFFFAOYSA-N
Formula:	C20H38O5
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)OCCOC
Mol. weight [g/mol]:	358.51

Physical Properties

Property code	Value	Unit	Source
gf	-455.32	kJ/mol	Joback Method
hf	-1077.95	kJ/mol	Joback Method
hfus	54.32	kJ/mol	Joback Method
hvap	80.84	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.810		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	2509.00		NIST Webbook
tb	832.00	K	Joback Method
tc	1019.41	K	Joback Method
tf	481.71	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.84	J/molxK	832.00	Joback Method
cpg	1018.88	J/molxK	863.24	Joback Method
cpg	1035.80	J/molxK	894.47	Joback Method
cpg	1051.59	J/molxK	925.71	Joback Method
cpg	1066.26	J/molxK	956.94	Joback Method
cpg	1079.84	J/molxK	988.18	Joback Method
cpg	1092.31	J/molxK	1019.41	Joback Method
dvisc	0.0005736	Paxs	481.71	Joback Method
dvisc	0.0002891	Paxs	540.09	Joback Method

dvisc	0.0001666	Paxs	598.47	Joback Method
dvisc	0.0001059	Paxs	656.86	Joback Method
dvisc	0.0000725	Paxs	715.24	Joback Method
dvisc	0.0000525	Paxs	773.62	Joback Method
dvisc	0.0000398	Paxs	832.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U355759&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

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