

Sebacic acid, di(2-methoxyethyl) ester

Inchi: InChI=1S/C16H30O6/c1-19-11-13-21-15(17)9-7-5-3-4-6-8-10-16(18)22-14-12-20-2/h3-14
InchiKey: JGDURTCBAJOZDJ-UHFFFAOYSA-N
Formula: C16H30O6
SMILES: COCCOC(=O)CCCCCCCCC(=O)OCCOC
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-594.00	kJ/mol	Joback Method
hf	-1127.61	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	74.34	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.486		Crippen Method
mcvol	262.920	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2257.00		NIST Webbook
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tb	762.90	K	Joback Method
tc	942.20	K	Joback Method
tf	458.86	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.67	J/molxK	762.90	Joback Method
cpg	865.50	J/molxK	912.32	Joback Method
cpg	852.97	J/molxK	882.43	Joback Method
cpg	839.51	J/molxK	852.55	Joback Method
cpg	825.14	J/molxK	822.67	Joback Method
cpg	809.86	J/molxK	792.78	Joback Method
cpg	877.09	J/molxK	942.20	Joback Method
dvisc	0.0000532	Paxs	762.90	Joback Method

dvisc	0.0000691	Paxs	712.23	Joback Method
dvisc	0.0000933	Paxs	661.55	Joback Method
dvisc	0.0001325	Paxs	610.88	Joback Method
dvisc	0.0002005	Paxs	560.21	Joback Method
dvisc	0.0003295	Paxs	509.53	Joback Method
dvisc	0.0006043	Paxs	458.86	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=U355770&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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