

Sebacic acid, but-3-enyl propyl ester

Inchi:	InChI=1S/C17H30O4/c1-3-5-15-21-17(19)13-11-9-7-6-8-10-12-16(18)20-14-4-2/h3H,1,4-
InchiKey:	CDBXNNSSKHGMMC-UHFFFAOYSA-N
Formula:	C17H30O4
SMILES:	C=CCCOC(=O)CCCCCCCCC(=O)OCCC
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	-287.74	kJ/mol	Joback Method
hf	-758.38	kJ/mol	Joback Method
hfus	44.08	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.180		Crippen Method
mvol	260.970	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
tb	737.62	K	Joback Method
tc	916.09	K	Joback Method
tf	423.91	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.83	J/molxK	737.62	Joback Method
cpg	782.30	J/molxK	767.36	Joback Method
cpg	797.92	J/molxK	797.11	Joback Method
cpg	812.71	J/molxK	826.85	Joback Method
cpg	826.68	J/molxK	856.60	Joback Method
cpg	839.84	J/molxK	886.34	Joback Method
cpg	852.20	J/molxK	916.09	Joback Method
dvisc	0.0011463	Paxs	423.91	Joback Method

dvisc	0.0005872	Paxs	476.20	Joback Method
dvisc	0.0003434	Paxs	528.48	Joback Method
dvisc	0.0002212	Paxs	580.77	Joback Method
dvisc	0.0001532	Paxs	633.05	Joback Method
dvisc	0.0001122	Paxs	685.34	Joback Method
dvisc	0.0000859	Paxs	737.62	Joback Method

Sources

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=U356082&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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