

Sebacic acid, but-3-enyl tetradecyl ester

Inchi:

InChI=1S/C28H52O4/c1-3-5-7-8-9-10-11-12-13-16-19-22-26-32-28(30)24-21-18-15-14-1

InchiKey:

JNPXKACTWMDULZ-UHFFFAOYSA-N

Formula:

C28H52O4

SMILES:

C=CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCCCC

Mol. weight [g/mol]:

452.71

Physical Properties

Property code	Value	Unit	Source
gf	-195.12	kJ/mol	Joback Method
hf	-985.42	kJ/mol	Joback Method
hfus	72.57	kJ/mol	Joback Method
hvap	95.56	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.471		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	702.84	kPa	Joback Method
rinpol	3167.00		NIST Webbook
rinpol	3167.00		NIST Webbook
tb	989.30	K	Joback Method
tc	1226.22	K	Joback Method
tf	547.88	K	Joback Method
vc	1.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1444.22	J/mol×K	989.30	Joback Method
cpg	1536.48	J/mol×K	1186.74	Joback Method
cpg	1521.51	J/mol×K	1147.25	Joback Method
cpg	1504.89	J/mol×K	1107.76	Joback Method
cpg	1486.51	J/mol×K	1068.27	Joback Method
cpg	1466.32	J/mol×K	1028.79	Joback Method
cpg	1549.85	J/mol×K	1226.22	Joback Method
dvisc	0.0000171	Pa×s	989.30	Joback Method

dvisc	0.0000229	Pa×s	915.73	Joback Method
dvisc	0.0000323	Pa×s	842.16	Joback Method
dvisc	0.0000488	Pa×s	768.59	Joback Method
dvisc	0.0000803	Pa×s	695.02	Joback Method
dvisc	0.0001487	Pa×s	621.45	Joback Method
dvisc	0.0003251	Pa×s	547.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356094&Units=SI
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

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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