

Sebacic acid, but-3-enyl pentadecyl ester

Inchi:	InChI=1S/C29H54O4/c1-3-5-7-8-9-10-11-12-13-14-17-20-23-27-33-29(31)25-22-19-16-1
InchiKey:	QWUVIJUUGFNXQQ-UHFFFAOYSA-N
Formula:	C29H54O4
SMILES:	C=CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	466.74

Physical Properties

Property code	Value	Unit	Source
gf	-186.70	kJ/mol	Joback Method
hf	-1006.06	kJ/mol	Joback Method
hfus	75.16	kJ/mol	Joback Method
hvap	97.79	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.861		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	668.39	kPa	Joback Method
rinsol	3266.00		NIST Webbook
tb	1012.18	K	Joback Method
tc	1261.06	K	Joback Method
tf	559.15	K	Joback Method
vc	1.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1509.12	J/molxK	1012.18	Joback Method
cpg	1531.97	J/molxK	1053.66	Joback Method
cpg	1552.72	J/molxK	1095.14	Joback Method
cpg	1571.47	J/molxK	1136.62	Joback Method
cpg	1588.31	J/molxK	1178.10	Joback Method
cpg	1603.33	J/molxK	1219.58	Joback Method
cpg	1616.64	J/molxK	1261.06	Joback Method
dvisc	0.0002845	Paxs	559.15	Joback Method
dvisc	0.0001291	Paxs	634.66	Joback Method

dvisc	0.0000693	Paxs	710.16	Joback Method
dvisc	0.0000420	Paxs	785.67	Joback Method
dvisc	0.0000277	Paxs	861.17	Joback Method
dvisc	0.0000196	Paxs	936.68	Joback Method
dvisc	0.0000146	Paxs	1012.18	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=U356095&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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