

Sebacic acid, octyl tridec-2-ynyl ester

Inchi: InChI=1S/C31H56O4/c1-3-5-7-9-11-12-13-14-17-21-25-29-35-31(33)27-23-19-16-15-18-
InchiKey: YIOHISSJXZJVGC-UHFFFAOYSA-N
Formula: C31H56O4
SMILES: CCCCCCCCCC#CCOC(=O)CCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
gf	-54.90	kJ/mol	Joback Method
hf	-900.47	kJ/mol	Joback Method
hfus	84.74	kJ/mol	Joback Method
hvap	105.06	kJ/mol	Joback Method
log10ws	-10.32		Crippen Method
logp	9.088		Crippen Method
mcvol	453.930	ml/mol	McGowan Method
pc	643.53	kPa	Joback Method
rinpol	3534.00		NIST Webbook
tb	1070.26	K	Joback Method
tc	1338.77	K	Joback Method
tf	689.55	K	Joback Method
vc	1.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1612.93	J/mol×K	1070.26	Joback Method
cpg	1635.32	J/mol×K	1115.01	Joback Method
cpg	1655.25	J/mol×K	1159.76	Joback Method
cpg	1672.85	J/mol×K	1204.52	Joback Method
cpg	1688.22	J/mol×K	1249.27	Joback Method
cpg	1701.48	J/mol×K	1294.02	Joback Method
cpg	1712.74	J/mol×K	1338.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355862&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
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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