

Sebacic acid, tetrahydrofurfuryl tridecyl ester

Inchi:	InChI=1S/C28H52O5/c1-2-3-4-5-6-7-8-9-12-15-18-23-32-27(29)21-16-13-10-11-14-17-22
InchiKey:	CSDZPVKESHUTPY-UHFFFAOYSA-N
Formula:	C28H52O5
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	468.71

Physical Properties

Property code	Value	Unit	Source
gf	-332.53	kJ/mol	Joback Method
hf	-1182.37	kJ/mol	Joback Method
hfus	75.76	kJ/mol	Joback Method
hvap	101.00	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.684		Crippen Method
mcvol	415.270	ml/mol	McGowan Method
pc	753.50	kPa	Joback Method
rinpola	3421.00		NIST Webbook
tb	1034.85	K	Joback Method
tc	1279.66	K	Joback Method
tf	587.11	K	Joback Method
vc	1.613	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1501.08	J/molxK	1034.85	Joback Method
cpg	1521.71	J/molxK	1075.65	Joback Method
cpg	1540.26	J/molxK	1116.45	Joback Method
cpg	1556.81	J/molxK	1157.26	Joback Method
cpg	1571.45	J/molxK	1198.06	Joback Method
cpg	1584.28	J/molxK	1238.86	Joback Method
cpg	1595.40	J/molxK	1279.66	Joback Method
dvisc	0.0003323	Paxs	587.11	Joback Method
dvisc	0.0001595	Paxs	661.73	Joback Method

dvisc	0.0000888	Paxs	736.36	Joback Method
dvisc	0.0000551	Paxs	810.98	Joback Method
dvisc	0.0000371	Paxs	885.60	Joback Method
dvisc	0.0000265	Paxs	960.23	Joback Method
dvisc	0.0000199	Paxs	1034.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355729&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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