

Sebacic acid, tetrahydrofurfuryl octyl ester

Inchi: InChI=1S/C23H42O5/c1-2-3-4-5-10-13-18-27-22(24)16-11-8-6-7-9-12-17-23(25)28-20-21
InchiKey: WIFJXWUISPPFCB-UHFFFAOYSA-N
Formula: C23H42O5
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]: 398.58

Physical Properties

Property code	Value	Unit	Source
gf	-374.63	kJ/mol	Joback Method
hf	-1079.17	kJ/mol	Joback Method
hfus	62.81	kJ/mol	Joback Method
hvap	89.87	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.733		Crippen Method
mcvol	344.820	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2913.00		NIST Webbook
rinpol	2913.00		NIST Webbook
tb	920.45	K	Joback Method
tc	1126.92	K	Joback Method
tf	530.76	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.69	J/mol×K	920.45	Joback Method
cpg	1201.40	J/mol×K	954.86	Joback Method
cpg	1218.68	J/mol×K	989.27	Joback Method
cpg	1234.56	J/mol×K	1023.68	Joback Method
cpg	1249.08	J/mol×K	1058.09	Joback Method
cpg	1262.29	J/mol×K	1092.50	Joback Method
cpg	1274.22	J/mol×K	1126.92	Joback Method
dvisc	0.0006283	Pa×s	530.76	Joback Method

dvisc	0.0003157	Pa×s	595.71	Joback Method
dvisc	0.0001816	Pa×s	660.66	Joback Method
dvisc	0.0001153	Pa×s	725.61	Joback Method
dvisc	0.0000789	Pa×s	790.55	Joback Method
dvisc	0.0000572	Pa×s	855.50	Joback Method
dvisc	0.0000434	Pa×s	920.45	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=U355724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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