

Sebacic acid, tetrahydrofurfuryl isobutyl ester

Inchi:	InChI=1S/C19H34O5/c1-16(2)14-23-18(20)11-7-5-3-4-6-8-12-19(21)24-15-17-10-9-13-22
InchiKey:	WRBACYGWQMVWFF-UHFFFAOYSA-N
Formula:	C19H34O5
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	342.47

Physical Properties

Property code	Value	Unit	Source
gf	-410.75	kJ/mol	Joback Method
hf	-1001.89	kJ/mol	Joback Method
hfus	48.93	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.029		Crippen Method
mvol	288.460	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	828.49	K	Joback Method
tc	1023.86	K	Joback Method
tf	470.68	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.15	J/molxK	828.49	Joback Method
cpg	954.98	J/molxK	861.05	Joback Method
cpg	971.62	J/molxK	893.61	Joback Method
cpg	987.09	J/molxK	926.17	Joback Method
cpg	1001.41	J/molxK	958.73	Joback Method
cpg	1014.61	J/molxK	991.30	Joback Method
cpg	1026.71	J/molxK	1023.86	Joback Method
dvisc	0.0011404	Paxs	470.68	Joback Method

dvisc	0.0005554	Paxs	530.32	Joback Method
dvisc	0.0003128	Paxs	589.95	Joback Method
dvisc	0.0001958	Paxs	649.59	Joback Method
dvisc	0.0001326	Paxs	709.22	Joback Method
dvisc	0.0000954	Paxs	768.86	Joback Method
dvisc	0.0000719	Paxs	828.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355719&Units=SI
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

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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