

Succinic acid, phenethyl 2-ethoxyethyl ester

Inchi:	InChI=1S/C16H22O5/c1-2-19-12-13-21-16(18)9-8-15(17)20-11-10-14-6-4-3-5-7-14/h3-7H
InchiKey:	PNARWVJTTQDQNX-UHFFFAOYSA-N
Formula:	C16H22O5
SMILES:	CCOCCOC(=O)CCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	294.34

Physical Properties

Property code	Value	Unit	Source
gf	-376.59	kJ/mol	Joback Method
hf	-758.86	kJ/mol	Joback Method
hfus	38.00	kJ/mol	Joback Method
hvap	74.21	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.132		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2189.00		NIST Webbook
tb	767.16	K	Joback Method
tc	967.46	K	Joback Method
tf	463.05	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.14	J/molxK	767.16	Joback Method
cpg	691.99	J/molxK	800.54	Joback Method
cpg	705.82	J/molxK	833.93	Joback Method
cpg	718.66	J/molxK	867.31	Joback Method
cpg	730.48	J/molxK	900.69	Joback Method
cpg	741.32	J/molxK	934.07	Joback Method
cpg	751.15	J/molxK	967.46	Joback Method
dvisc	0.0007211	Paxs	463.05	Joback Method
dvisc	0.0004049	Paxs	513.73	Joback Method

dvisc	0.0002521	Paxs	564.42	Joback Method
dvisc	0.0001698	Paxs	615.11	Joback Method
dvisc	0.0001214	Paxs	665.79	Joback Method
dvisc	0.0000910	Paxs	716.47	Joback Method
dvisc	0.0000709	Paxs	767.16	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=U358003&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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