

Succinic acid, 3,4-dimethylphenyl 2-ethoxyethyl ester

Inchi:	InChI=1S/C16H22O5/c1-4-19-9-10-20-15(17)7-8-16(18)21-14-6-5-12(2)13(3)11-14/h5-6,
InchiKey:	FXPWXYOTWWHLLB-UHFFFAOYSA-N
Formula:	C16H22O5
SMILES:	CCOCCOC(=O)CCC(=O)Oc1ccc(C)c(C)c1
Mol. weight [g/mol]:	294.34

Physical Properties

Property code	Value	Unit	Source
gf	-395.85	kJ/mol	Joback Method
hf	-781.80	kJ/mol	Joback Method
hfus	37.22	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.569		Crippen Method
mvol	233.290	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2235.00		NIST Webbook
tb	777.12	K	Joback Method
tc	979.03	K	Joback Method
tf	488.09	K	Joback Method
vc	0.889	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.43	J/molxK	777.12	Joback Method
cpg	738.65	J/molxK	945.38	Joback Method
cpg	728.03	J/molxK	911.73	Joback Method
cpg	716.39	J/molxK	878.08	Joback Method
cpg	703.73	J/molxK	844.42	Joback Method
cpg	690.08	J/molxK	810.77	Joback Method
cpg	748.25	J/molxK	979.03	Joback Method
dvisc	0.0000717	Paxs	777.12	Joback Method
dvisc	0.0000895	Paxs	728.95	Joback Method

dvisc	0.0001152	Paxs	680.78	Joback Method
dvisc	0.0001543	Paxs	632.61	Joback Method
dvisc	0.0002166	Paxs	584.43	Joback Method
dvisc	0.0003234	Paxs	536.26	Joback Method
dvisc	0.0005225	Paxs	488.09	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=U357563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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