Sebacic acid, 3-ethylphenyl propyl ester

Inchi: InChI=1S/C21H32O4/c1-3-16-24-20(22)14-9-7-5-6-8-10-15-21(23)25-19-13-11-12-18(4-2
InchiKey: CPCHAFJEXFCEKT-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)Oc1cccc(CC)c1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-239.12	kJ/mol	Joback Method
hf	-741.31	kJ/mol	Joback Method
hfus	49.37	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.228		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1252.15	kPa	Joback Method
rinpol	2597.00		NIST Webbook
tb	864.12	K	Joback Method
tc	1065.34	K	Joback Method
tf	509.69	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.16	J/mol×K	864.12	Joback Method
cpg	953.50	J/mol×K	897.66	Joback Method
cpg	968.67	J/mol×K	931.19	Joback Method
cpg	982.68	J/mol×K	964.73	Joback Method
cpg	995.57	J/mol×K	998.27	Joback Method
cpg	1007.37	J/mol×K	1031.80	Joback Method
cpg	1018.08	J/mol×K	1065.34	Joback Method
dvisc	0.0005353	Pa×s	509.69	Joback Method
dvisc	0.0002901	Pa×s	568.76	Joback Method

dvisc	0.0001764	Pa×s	627.83	Joback Method
dvisc	0.0001169	Pa×s	686.90	Joback Method
dvisc	0.0000826	Pa×s	745.98	Joback Method
dvisc	0.0000615	Pa×s	805.05	Joback Method
dvisc	0.0000476	Pa×s	864.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355233&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/19-092-9/Sebacic-acid-3-ethylphenyl-propyl-ester.pdf
Generated by Cheméo on 2024-04-29 12:40:11.302099812 +0000 UTC m=+16683660.222677140.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.