

Glutaric acid, ethyl 2-naphthyl ester

Inchi: InChI=1S/C17H18O4/c1-2-20-16(18)8-5-9-17(19)21-15-11-10-13-6-3-4-7-14(13)12-15/h3
InchiKey: PYIGHIPEXXPIQQ-UHFFFAOYSA-N
Formula: C17H18O4
SMILES: CCOC(=O)CCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 286.32

Physical Properties

Property code	Value	Unit	Source
gf	-166.15	kJ/mol	Joback Method
hf	-467.68	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	76.33	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.479		Crippen Method
mcvol	222.050	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	2422.00		NIST Webbook
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tb	791.58	K	Joback Method
tc	1010.50	K	Joback Method
tf	497.31	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.40	J/molxK	791.58	Joback Method
cpg	647.17	J/molxK	828.07	Joback Method
cpg	659.92	J/molxK	864.55	Joback Method
cpg	671.70	J/molxK	901.04	Joback Method
cpg	682.54	J/molxK	937.53	Joback Method
cpg	692.49	J/molxK	974.01	Joback Method
cpg	701.60	J/molxK	1010.50	Joback Method
dvisc	0.0008938	Paxs	497.31	Joback Method

dvisc	0.0005867	Paxs	546.36	Joback Method
dvisc	0.0004128	Paxs	595.40	Joback Method
dvisc	0.0003064	Paxs	644.45	Joback Method
dvisc	0.0002372	Paxs	693.49	Joback Method
dvisc	0.0001899	Paxs	742.54	Joback Method
dvisc	0.0001563	Paxs	791.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358776&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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