

Glutaric acid, 1-naphthyl propyl ester

Inchi:	InChI=1S/C18H20O4/c1-2-13-21-17(19)11-6-12-18(20)22-16-10-5-8-14-7-3-4-9-15(14)16
InchiKey:	CJSOUXLHNAATKV-UHFFFAOYSA-N
Formula:	C18H20O4
SMILES:	CCCOC(=O)CCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	300.35

Physical Properties

Property code	Value	Unit	Source
gf	-157.73	kJ/mol	Joback Method
hf	-488.32	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.869		Crippen Method
mvol	236.140	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	2487.00		NIST Webbook
tb	814.46	K	Joback Method
tc	1031.08	K	Joback Method
tf	508.58	K	Joback Method
vc	0.905	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.97	J/molxK	814.46	Joback Method
cpg	749.31	J/molxK	994.98	Joback Method
cpg	739.13	J/molxK	958.87	Joback Method
cpg	728.05	J/molxK	922.77	Joback Method
cpg	716.02	J/molxK	886.67	Joback Method
cpg	703.01	J/molxK	850.56	Joback Method
cpg	758.63	J/molxK	1031.08	Joback Method
dvisc	0.0001389	Paxs	814.46	Joback Method
dvisc	0.0001695	Paxs	763.48	Joback Method

dvisc	0.0002127	Paxs	712.50	Joback Method
dvisc	0.0002766	Paxs	661.52	Joback Method
dvisc	0.0003757	Paxs	610.54	Joback Method
dvisc	0.0005396	Paxs	559.56	Joback Method
dvisc	0.0008334	Paxs	508.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358763&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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