

Glutaric acid, isoheptyl 1-naphthyl ester

Inchi:	InChI=1S/C21H26O4/c1-16(2)8-7-15-24-20(22)13-6-14-21(23)25-19-12-5-10-17-9-3-4-11
InchiKey:	ZVZYLLZRPAFOMO-UHFFFAOYSA-N
Formula:	C21H26O4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	342.43

Physical Properties

Property code	Value	Unit	Source
gf	-134.91	kJ/mol	Joback Method
hf	-555.52	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.895		Crippen Method
mcvol	278.410	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2760.00		NIST Webbook
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tb	882.66	K	Joback Method
tc	1098.28	K	Joback Method
tf	527.39	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.57	J/mol×K	882.66	Joback Method
cpg	876.41	J/mol×K	918.60	Joback Method
cpg	890.13	J/mol×K	954.53	Joback Method
cpg	902.78	J/mol×K	990.47	Joback Method
cpg	914.42	J/mol×K	1026.41	Joback Method
cpg	925.10	J/mol×K	1062.35	Joback Method
cpg	934.88	J/mol×K	1098.28	Joback Method
dvisc	0.0007083	Pa×s	527.39	Joback Method

dvisc	0.0004187	Pa×s	586.60	Joback Method
dvisc	0.0002725	Pa×s	645.81	Joback Method
dvisc	0.0001907	Pa×s	705.03	Joback Method
dvisc	0.0001410	Pa×s	764.24	Joback Method
dvisc	0.0001089	Pa×s	823.45	Joback Method
dvisc	0.0000871	Pa×s	882.66	Joback Method

Sources

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=U358767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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