

Glutaric acid, naphth-2-ylmethyl isobutyl ester

Inchi:	InChI=1S/C20H24O4/c1-15(2)13-23-19(21)8-5-9-20(22)24-14-16-10-11-17-6-3-4-7-18(17)
InchiKey:	XEAJYTJFIKOCBQ-UHFFFAOYSA-N
Formula:	C20H24O4
SMILES:	CC(C)COC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	328.40

Physical Properties

Property code	Value	Unit	Source
gf	-143.33	kJ/mol	Joback Method
hf	-534.88	kJ/mol	Joback Method
hfus	40.28	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.253		Crippen Method
mvol	264.320	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2654.00		NIST Webbook
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tb	859.78	K	Joback Method
tc	1076.09	K	Joback Method
tf	516.12	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.39	J/molxK	859.78	Joback Method
cpg	818.05	J/molxK	895.83	Joback Method
cpg	831.60	J/molxK	931.88	Joback Method
cpg	844.10	J/molxK	967.94	Joback Method
cpg	855.60	J/molxK	1003.99	Joback Method
cpg	866.15	J/molxK	1040.04	Joback Method
cpg	875.79	J/molxK	1076.09	Joback Method
dvisc	0.0007738	Paxs	516.12	Joback Method

dvisc	0.0004631	Paxs	573.40	Joback Method
dvisc	0.0003042	Paxs	630.67	Joback Method
dvisc	0.0002143	Paxs	687.95	Joback Method
dvisc	0.0001594	Paxs	745.23	Joback Method
dvisc	0.0001236	Paxs	802.50	Joback Method
dvisc	0.0000992	Paxs	859.78	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=U391505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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