

Glutaric acid, naphth-2-ylmethyl 2-ethylbutyl ester

Inchi:	InChI=1S/C22H28O4/c1-3-17(4-2)15-25-21(23)10-7-11-22(24)26-16-18-12-13-19-8-5-6-9
InchiKey:	XIKIAJWZZCMVKC-UHFFFAOYSA-N
Formula:	C22H28O4
SMILES:	CCC(CC)COC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	356.46

Physical Properties

Property code	Value	Unit	Source
gf	-126.49	kJ/mol	Joback Method
hf	-576.16	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	87.07	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.033		Crippen Method
mvol	292.500	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2855.00		NIST Webbook
rinpol	2855.00		NIST Webbook
tb	905.54	K	Joback Method
tc	1121.21	K	Joback Method
tf	538.66	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.50	J/molxK	905.54	Joback Method
cpg	984.77	J/molxK	1085.26	Joback Method
cpg	973.97	J/molxK	1049.32	Joback Method
cpg	962.20	J/molxK	1013.37	Joback Method
cpg	949.40	J/molxK	977.43	Joback Method
cpg	935.52	J/molxK	941.48	Joback Method
cpg	994.66	J/molxK	1121.21	Joback Method
dvisc	0.0000762	Paxs	905.54	Joback Method

dvisc	0.0000956	Paxs	844.39	Joback Method
dvisc	0.0001243	Paxs	783.25	Joback Method
dvisc	0.0001690	Paxs	722.10	Joback Method
dvisc	0.0002432	Paxs	660.95	Joback Method
dvisc	0.0003770	Paxs	599.81	Joback Method
dvisc	0.0006454	Paxs	538.66	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=U391678&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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