

Glutaric acid, hex-2-en-1-yl naphth-2-ylmethyl ester

Inchi:	InChI=1S/C22H26O4/c1-2-3-4-7-15-25-21(23)11-8-12-22(24)26-17-18-13-14-19-9-5-6-10
InchiKey:	ZNJDIBPNKZFHHG-QPJXVBHSA-N
Formula:	C22H26O4
SMILES:	CCCC=CCOC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-43.83	kJ/mol	Joback Method
hf	-453.66	kJ/mol	Joback Method
hfus	49.18	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	4.953		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpola	2881.00		NIST Webbook
tb	910.14	K	Joback Method
tc	1128.19	K	Joback Method
tf	548.58	K	Joback Method
vc	1.109	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.15	J/molxK	910.14	Joback Method
cpg	955.78	J/molxK	1091.85	Joback Method
cpg	944.79	J/molxK	1055.51	Joback Method
cpg	933.00	J/molxK	1019.16	Joback Method
cpg	920.34	J/molxK	982.82	Joback Method
cpg	906.75	J/molxK	946.48	Joback Method
cpg	966.06	J/molxK	1128.19	Joback Method
dvisc	0.0000731	Paxs	910.14	Joback Method
dvisc	0.0000908	Paxs	849.88	Joback Method

dvisc	0.0001165	Paxs	789.62	Joback Method
dvisc	0.0001558	Paxs	729.36	Joback Method
dvisc	0.0002196	Paxs	669.10	Joback Method
dvisc	0.0003313	Paxs	608.84	Joback Method
dvisc	0.0005470	Paxs	548.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405342&Units=SI

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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