

Glutaric acid, 2-ethylhexyl 3-nitrobenzyl ester

Inchi:	InChI=1S/C20H29NO6/c1-3-5-8-16(4-2)14-26-19(22)11-7-12-20(23)27-15-17-9-6-10-18(
InchiKey:	PBGOGZPUCAKXPO-UHFFFAOYSA-N
Formula:	C20H29NO6
SMILES:	CCCCC(CC)COC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	379.45

Physical Properties

Property code	Value	Unit	Source
gf	-214.43	kJ/mol	Joback Method
hf	-736.71	kJ/mol	Joback Method
hfus	54.62	kJ/mol	Joback Method
hvap	97.57	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.568		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpola	2855.00		NIST Webbook
rinpola	2855.00		NIST Webbook
tb	992.64	K	Joback Method
tc	1219.48	K	Joback Method
tf	627.03	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.83	J/molxK	992.64	Joback Method
cpg	1001.42	J/molxK	1030.45	Joback Method
cpg	1012.62	J/molxK	1068.25	Joback Method
cpg	1022.49	J/molxK	1106.06	Joback Method
cpg	1031.05	J/molxK	1143.87	Joback Method
cpg	1038.35	J/molxK	1181.67	Joback Method
cpg	1044.43	J/molxK	1219.48	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=U393357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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