

Glutaric acid, 8-chlorooctyl (2-naphthyl)methyl ester

Inchi: InChI=1S/C24H31ClO4/c25-16-7-3-1-2-4-8-17-28-23(26)12-9-13-24(27)29-19-20-14-15-2
InchiKey: OOXSBHRRSJWKD-UHFFFAOYSA-N
Formula: C24H31ClO4
SMILES: O=C(CCCC(=O)OCc1ccc2ccccc2c1)OCCCCCCCCI
Mol. weight [g/mol]: 418.95

Physical Properties

Property code	Value	Unit	Source
gf	-119.14	kJ/mol	Joback Method
hf	-627.90	kJ/mol	Joback Method
hfus	58.36	kJ/mol	Joback Method
hvap	96.29	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.176		Crippen Method
mvol	332.920	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinpol	3424.00		NIST Webbook
rinpol	3424.00		NIST Webbook
tb	989.17	K	Joback Method
tc	1212.87	K	Joback Method
tf	606.12	K	Joback Method
vc	1.290	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.19	J/molxK	989.17	Joback Method
cpg	1125.11	J/molxK	1175.59	Joback Method
cpg	1114.92	J/molxK	1138.30	Joback Method
cpg	1103.81	J/molxK	1101.02	Joback Method
cpg	1091.70	J/molxK	1063.74	Joback Method
cpg	1078.52	J/molxK	1026.45	Joback Method
cpg	1134.45	J/molxK	1212.87	Joback Method
dvisc	0.0000544	Paxs	989.17	Joback Method

dvisc	0.0000678	Paxs	925.33	Joback Method
dvisc	0.0000874	Paxs	861.49	Joback Method
dvisc	0.0001173	Paxs	797.64	Joback Method
dvisc	0.0001656	Paxs	733.80	Joback Method
dvisc	0.0002497	Paxs	669.96	Joback Method
dvisc	0.0004105	Paxs	606.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392209&Units=SI
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

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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