Glutaric acid, monoamide, N-(2-octyl)-, heptyl ester

Inchi: InChI=1S/C20H39NO3/c1-4-6-8-10-12-17-24-20(23)16-13-15-19(22)21-18(3)14-11-9-7-5

InchiKey: XIZLAUNXFHGULO-UHFFFAOYSA-N

Formula: C20H39NO3

SMILES: CCCCCCCOC(=O)CCCC(=O)NC(C)CCCCCC

Mol. weight [g/mol]: 341.53

Physical Properties

Property code	Value	Unit	Source
gf	-158.37	kJ/mol	Joback Method
hf	-765.32	kJ/mol	Joback Method
hfus	53.52	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.145		Crippen Method
mcvol	311.650	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook
tb	836.89	K	Joback Method
tc	1026.30	K	Joback Method
tf	474.91	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.70	J/mol×K	836.89	Joback Method
cpg	1020.82	J/mol×K	868.46	Joback Method
cpg	1037.87	J/mol×K	900.03	Joback Method
cpg	1053.88	J/mol×K	931.59	Joback Method
cpg	1068.87	J/mol×K	963.16	Joback Method
cpg	1082.87	J/mol×K	994.73	Joback Method
cpg	1095.92	J/mol×K	1026.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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