

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

Inchi:	InChI=1S/C16H31NO3/c1-4-6-7-8-10-14(3)17-15(18)11-9-12-16(19)20-13-5-2/h14H,4-13
InchiKey:	YXIDNOJQAZARPO-UHFFFAOYSA-N
Formula:	C16H31NO3
SMILES:	CCCCCCC(C)NC(=O)CCCC(=O)OCCC
Mol. weight [g/mol]:	285.42

Physical Properties

Property code	Value	Unit	Source
gf	-192.05	kJ/mol	Joback Method
hf	-682.76	kJ/mol	Joback Method
hfus	43.16	kJ/mol	Joback Method
hvap	73.16	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.585		Crippen Method
mcvol	255.290	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpola	2446.00		NIST Webbook
rinpola	2446.00		NIST Webbook
tb	745.37	K	Joback Method
tc	926.90	K	Joback Method
tf	429.83	K	Joback Method
vc	0.991	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.34	J/mol×K	745.37	Joback Method
cpg	781.92	J/mol×K	775.63	Joback Method
cpg	797.62	J/mol×K	805.88	Joback Method
cpg	812.46	J/mol×K	836.14	Joback Method
cpg	826.46	J/mol×K	866.39	Joback Method
cpg	839.64	J/mol×K	896.65	Joback Method
cpg	852.02	J/mol×K	926.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360851&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
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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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